



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:17 PM UTC

PDB ID : 5W0W / pdb\_00005w0w  
Title : Crystal structure of Protein Phosphatase 2A bound to TIPRL  
Authors : Wu, C.; Zheng, A.; Li, J.; Satyshur, K.; Xing, Y.  
Deposited on : 2017-06-01  
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

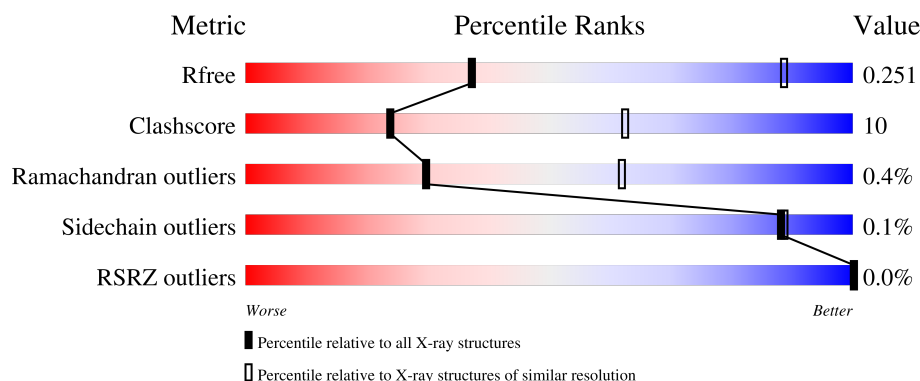
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1065 (3.96-3.64)                                      |
| Clashscore            | 190562                      | 1012 (3.94-3.66)                                      |
| Ramachandran outliers | 187476                      | 1048 (3.96-3.64)                                      |
| Sidechain outliers    | 187428                      | 1043 (3.96-3.64)                                      |
| RSRZ outliers         | 180081                      | 1064 (3.96-3.64)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 1   | A     | 585    | <br>81% 19% .   |
| 1   | D     | 585    | <br>80% 20% .   |
| 1   | G     | 585    | <br>76% 23%     |
| 1   | J     | 585    | <br>74% 25% .   |
| 2   | B     | 251    | <br>69% 17% 14% |

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| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 2   | E     | 251    | <br>66% 20% 14%  |
| 2   | H     | 251    | <br>69% 16% 14%  |
| 2   | K     | 251    | <br>61% 24% 14%  |
| 3   | C     | 311    | <br>77% 19% •    |
| 3   | F     | 311    | <br>69% 24% • 5% |
| 3   | I     | 311    | <br>70% 24% • 5% |
| 3   | L     | 311    | <br>71% 24% 5%   |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34732 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

| Mol | Chain | Residues | Atoms |      |     |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|----|---------|---------|-------|
| 1   | A     | 582      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 4535  | 2882 | 764 | 861 | 14 | 14 |         |         |       |
| 1   | D     | 582      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 4535  | 2882 | 764 | 861 | 14 | 14 |         |         |       |
| 1   | G     | 584      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 4551  | 2891 | 768 | 864 | 14 | 14 |         |         |       |
| 1   | J     | 580      | Total | C    | N   | O   | S  | Se | 0       | 0       | 0     |
|     |       |          | 4518  | 2870 | 762 | 858 | 14 | 14 |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 5       | GLY      | -      | expression tag | UNP P30153 |
| A     | 6       | SER      | -      | expression tag | UNP P30153 |
| A     | 7       | HIS      | -      | expression tag | UNP P30153 |
| A     | 8       | MSE      | -      | expression tag | UNP P30153 |
| D     | 5       | GLY      | -      | expression tag | UNP P30153 |
| D     | 6       | SER      | -      | expression tag | UNP P30153 |
| D     | 7       | HIS      | -      | expression tag | UNP P30153 |
| D     | 8       | MSE      | -      | expression tag | UNP P30153 |
| G     | 5       | GLY      | -      | expression tag | UNP P30153 |
| G     | 6       | SER      | -      | expression tag | UNP P30153 |
| G     | 7       | HIS      | -      | expression tag | UNP P30153 |
| G     | 8       | MSE      | -      | expression tag | UNP P30153 |
| J     | 5       | GLY      | -      | expression tag | UNP P30153 |
| J     | 6       | SER      | -      | expression tag | UNP P30153 |
| J     | 7       | HIS      | -      | expression tag | UNP P30153 |
| J     | 8       | MSE      | -      | expression tag | UNP P30153 |

- Molecule 2 is a protein called TIP41-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 216      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1754  | 1127 | 292 | 325 | 10 |         |         |       |
| 2   | E     | 215      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1746  | 1123 | 290 | 323 | 10 |         |         |       |
| 2   | H     | 215      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1743  | 1121 | 288 | 324 | 10 |         |         |       |
| 2   | K     | 215      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1747  | 1123 | 288 | 326 | 10 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 9       | GLY      | -      | expression tag | UNP Q8BH58 |
| B     | 10      | SER      | -      | expression tag | UNP Q8BH58 |
| B     | 11      | MET      | -      | expression tag | UNP Q8BH58 |
| E     | 9       | GLY      | -      | expression tag | UNP Q8BH58 |
| E     | 10      | SER      | -      | expression tag | UNP Q8BH58 |
| E     | 11      | MET      | -      | expression tag | UNP Q8BH58 |
| H     | 9       | GLY      | -      | expression tag | UNP Q8BH58 |
| H     | 10      | SER      | -      | expression tag | UNP Q8BH58 |
| H     | 11      | MET      | -      | expression tag | UNP Q8BH58 |
| K     | 9       | GLY      | -      | expression tag | UNP Q8BH58 |
| K     | 10      | SER      | -      | expression tag | UNP Q8BH58 |
| K     | 11      | MET      | -      | expression tag | UNP Q8BH58 |

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 298      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2424  | 1537 | 416 | 456 | 15 |         |         |       |
| 3   | F     | 296      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2387  | 1513 | 407 | 452 | 15 |         |         |       |
| 3   | I     | 296      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2394  | 1519 | 407 | 453 | 15 |         |         |       |
| 3   | L     | 296      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2394  | 1519 | 407 | 453 | 15 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -1      | GLY      | -      | expression tag | UNP P67775 |
| C     | 0       | SER      | -      | expression tag | UNP P67775 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | -1      | GLY      | -      | expression tag | UNP P67775 |
| F     | 0       | SER      | -      | expression tag | UNP P67775 |
| I     | -1      | GLY      | -      | expression tag | UNP P67775 |
| I     | 0       | SER      | -      | expression tag | UNP P67775 |
| L     | -1      | GLY      | -      | expression tag | UNP P67775 |
| L     | 0       | SER      | -      | expression tag | UNP P67775 |

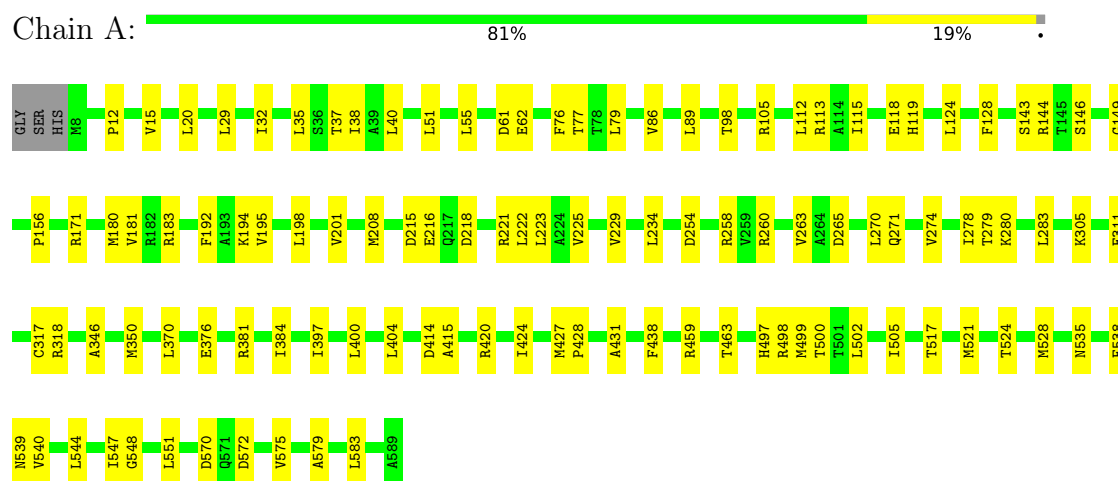
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4   | C     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |
| 4   | F     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |
| 4   | I     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |
| 4   | L     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |

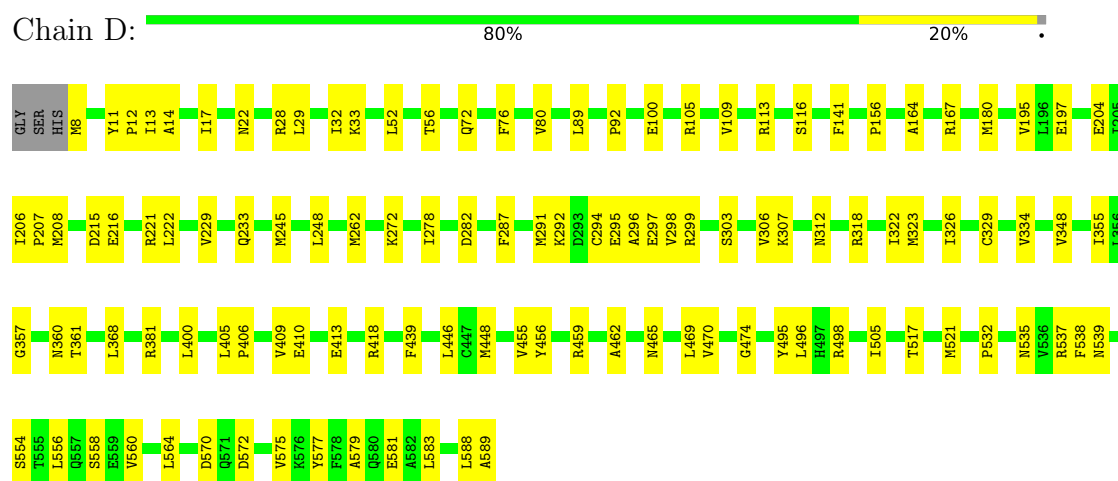
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

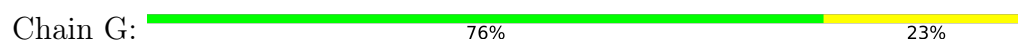
- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

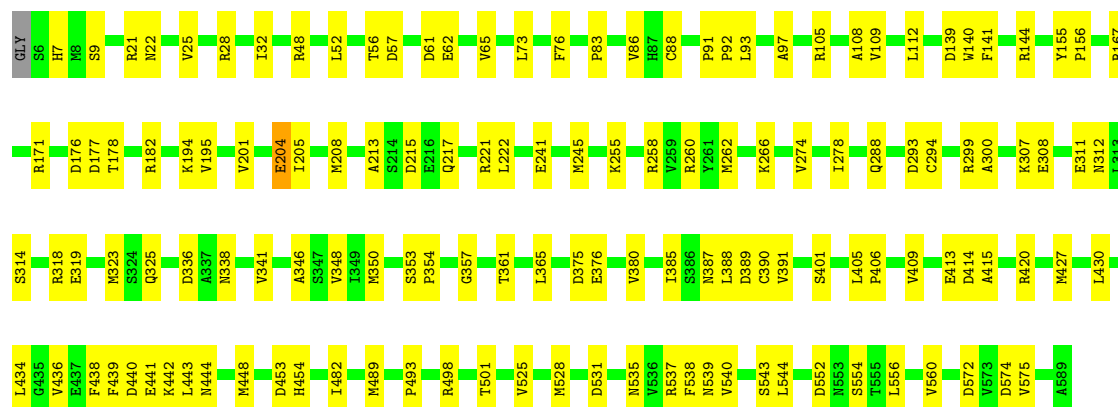


- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



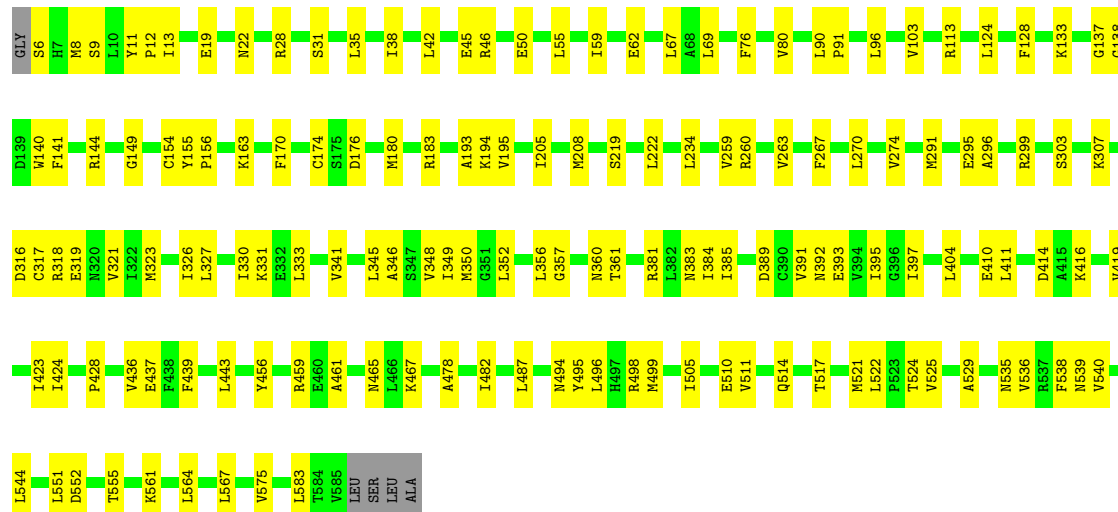
- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform





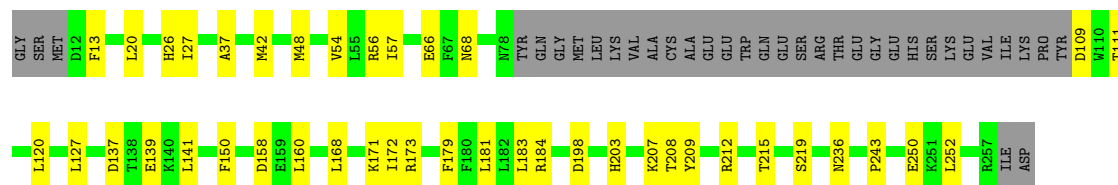
- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

Chain J: 74% 25% .



- Molecule 2: TIP41-like protein

Chain B: 69% 17% 14%

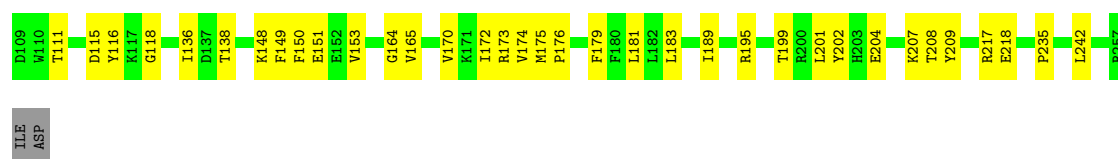


- Molecule 2: TIP41-like protein

Chain E: 66% 20% 14%

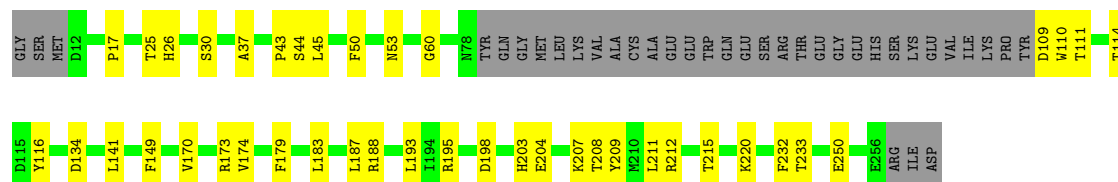






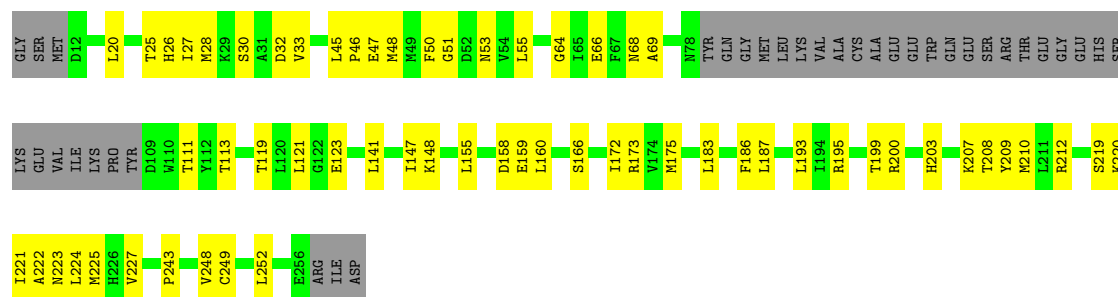
- Molecule 2: TIP41-like protein

Chain H:



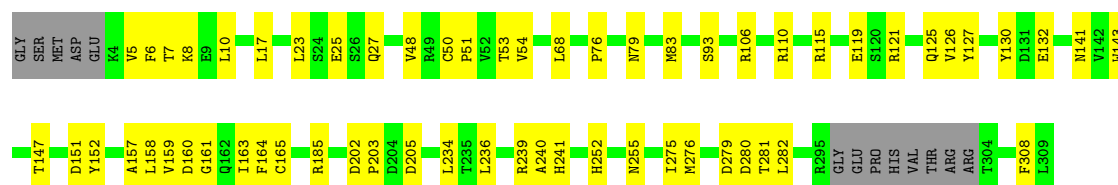
- Molecule 2: TIP41-like protein

Chain K:



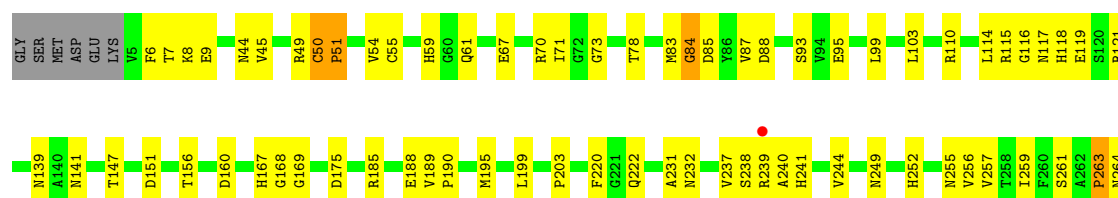
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain C:



- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

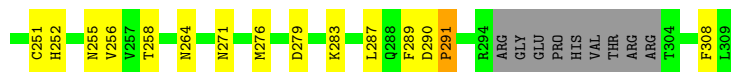
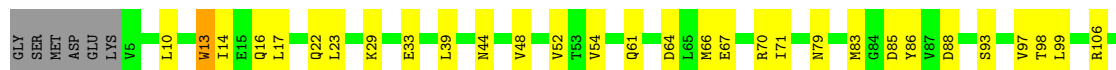
Chain F:





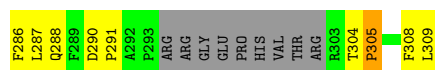
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain I: 70% 24% 5%



- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain L: 71% 24% 5%



## 4 Data and refinement statistics

| Property                                                                | Value                                                          | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------|------------------|
| Space group                                                             | P 32                                                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 150.98Å 150.98Å 285.50Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)                                                          | 49.42 – 3.80<br>49.42 – 3.80                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (49.42-3.80)<br>100.0 (49.42-3.80)                       | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.88                                                           | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.30 (at 3.57Å)                                                | Xtriage          |
| Refinement program                                                      | PHENIX (1.11.1_2575: ???)                                      | Depositor        |
| R, $R_{free}$                                                           | 0.197 , 0.246<br>0.205 , 0.251                                 | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5923 reflections (7.02%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 131.7                                                          | Xtriage          |
| Anisotropy                                                              | 0.294                                                          | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 142.8                                                   | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$    | Xtriage          |
| Estimated twinning fraction                                             | 0.054 for -h,-k,l<br>0.067 for h,-h-k,-l<br>0.058 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                           | EDS              |
| Total number of atoms                                                   | 34732                                                          | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 167.0                                                          | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | A     | 0.16         | 0/4596      | 0.36        | 0/6217         |
| 1   | D     | 0.16         | 0/4596      | 0.37        | 0/6217         |
| 1   | G     | 0.15         | 0/4612      | 0.37        | 0/6237         |
| 1   | J     | 0.19         | 0/4576      | 0.42        | 0/6186         |
| 2   | B     | 0.12         | 0/1794      | 0.34        | 0/2422         |
| 2   | E     | 0.14         | 0/1786      | 0.40        | 0/2411         |
| 2   | H     | 0.12         | 0/1783      | 0.36        | 0/2408         |
| 2   | K     | 0.16         | 0/1787      | 0.43        | 1/2413 (0.0%)  |
| 3   | C     | 0.14         | 0/2484      | 0.36        | 0/3366         |
| 3   | F     | 0.18         | 0/2445      | 0.43        | 0/3315         |
| 3   | I     | 0.15         | 0/2453      | 0.38        | 0/3326         |
| 3   | L     | 0.16         | 0/2453      | 0.42        | 0/3326         |
| All | All   | 0.16         | 0/35365     | 0.39        | 1/47844 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | K     | 51  | GLY  | N-CA-C | 5.36 | 115.09      | 110.21   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4535  | 0        | 4642     | 75      | 0            |
| 1   | D     | 4535  | 0        | 4642     | 86      | 0            |
| 1   | G     | 4551  | 0        | 4652     | 99      | 0            |
| 1   | J     | 4518  | 0        | 4615     | 113     | 0            |
| 2   | B     | 1754  | 0        | 1745     | 24      | 0            |
| 2   | E     | 1746  | 0        | 1739     | 37      | 0            |
| 2   | H     | 1743  | 0        | 1732     | 28      | 0            |
| 2   | K     | 1747  | 0        | 1736     | 43      | 0            |
| 3   | C     | 2424  | 0        | 2324     | 46      | 0            |
| 3   | F     | 2387  | 0        | 2285     | 67      | 0            |
| 3   | I     | 2394  | 0        | 2292     | 54      | 0            |
| 3   | L     | 2394  | 0        | 2292     | 61      | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 34732 | 0        | 34696    | 700     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (700) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:319:GLU:O    | 1:G:323:MSE:CE   | 1.94                     | 1.15              |
| 3:I:54:VAL:HG12  | 3:I:276:MET:HG2  | 1.41                     | 1.00              |
| 1:A:570:ASP:HB3  | 1:A:575:VAL:HG21 | 1.47                     | 0.95              |
| 1:J:22:ASN:O     | 1:J:28:ARG:NH2   | 2.01                     | 0.93              |
| 3:C:48:VAL:CG1   | 3:C:159:VAL:HG12 | 2.03                     | 0.89              |
| 3:L:87:VAL:HG23  | 3:L:93:SER:HB2   | 1.55                     | 0.88              |
| 3:L:160:ASP:HB3  | 3:L:282:LEU:HD11 | 1.55                     | 0.88              |
| 3:I:203:PRO:HD2  | 3:I:239:ARG:NH1  | 1.89                     | 0.88              |
| 2:K:27:ILE:HD12  | 2:K:48:MET:HA    | 1.55                     | 0.87              |
| 1:G:213:ALA:O    | 1:G:221:ARG:HG2  | 1.75                     | 0.86              |
| 1:G:319:GLU:O    | 1:G:323:MSE:HE1  | 1.77                     | 0.84              |
| 1:G:441:GLU:HG2  | 1:G:442:LYS:HG2  | 1.60                     | 0.84              |
| 3:C:48:VAL:HG13  | 3:C:159:VAL:HG12 | 1.56                     | 0.84              |
| 3:F:117:ASN:HD21 | 3:F:241:HIS:CE1  | 1.96                     | 0.83              |
| 3:I:203:PRO:HD2  | 3:I:239:ARG:HH12 | 1.44                     | 0.82              |
| 3:F:168:GLY:O    | 3:F:239:ARG:HD2  | 1.81                     | 0.81              |
| 3:F:67:GLU:OE1   | 3:F:70:ARG:NH2   | 2.13                     | 0.81              |
| 3:L:49:ARG:NH1   | 3:L:110:ARG:HH21 | 1.79                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:499:MSE:HE1  | 1:J:539:ASN:HD22 | 1.46                     | 0.80              |
| 1:J:389:ASP:O    | 1:J:393:GLU:OE1  | 2.01                     | 0.79              |
| 3:C:159:VAL:HG22 | 3:C:163:ILE:HB   | 1.64                     | 0.78              |
| 2:K:212:ARG:HG3  | 2:K:252:LEU:HD11 | 1.63                     | 0.78              |
| 3:I:54:VAL:CG1   | 3:I:276:MET:HG2  | 2.14                     | 0.77              |
| 2:K:141:LEU:O    | 2:K:173:ARG:NH1  | 2.17                     | 0.77              |
| 1:A:218:ASP:OD1  | 1:A:221:ARG:NH2  | 2.18                     | 0.77              |
| 2:H:37:ALA:HB2   | 2:H:45:LEU:HD22  | 1.69                     | 0.74              |
| 1:G:350:MSE:HG3  | 1:G:391:VAL:HG21 | 1.70                     | 0.74              |
| 1:A:215:ASP:O    | 1:A:221:ARG:NH1  | 2.21                     | 0.74              |
| 3:C:159:VAL:CG2  | 3:C:163:ILE:HB   | 2.18                     | 0.73              |
| 3:F:240:ALA:HB2  | 3:F:259:ILE:H    | 1.52                     | 0.73              |
| 2:E:217:ARG:NH1  | 2:E:242:LEU:O    | 2.21                     | 0.72              |
| 1:D:462:ALA:HA   | 1:D:465:ASN:ND2  | 2.05                     | 0.72              |
| 2:K:68:ASN:OD1   | 2:K:69:ALA:N     | 2.22                     | 0.72              |
| 1:J:295:GLU:O    | 1:J:299:ARG:NH1  | 2.23                     | 0.72              |
| 1:G:319:GLU:O    | 1:G:323:MSE:HE2  | 1.89                     | 0.72              |
| 3:C:93:SER:OG    | 3:C:132:GLU:OE1  | 2.07                     | 0.71              |
| 1:G:57:ASP:OD2   | 1:J:9:SER:OG     | 2.08                     | 0.71              |
| 1:J:113:ARG:NH1  | 1:J:149:GLY:O    | 2.23                     | 0.71              |
| 3:L:45:VAL:HG12  | 3:L:156:THR:OG1  | 1.91                     | 0.71              |
| 3:L:156:THR:HG22 | 3:L:166:LEU:HB2  | 1.73                     | 0.71              |
| 3:L:180:ILE:HD12 | 3:L:180:ILE:H    | 1.56                     | 0.70              |
| 3:L:304:THR:OG1  | 3:L:305:PRO:HD2  | 1.91                     | 0.70              |
| 3:I:13:TRP:O     | 3:I:16:GLN:N     | 2.23                     | 0.70              |
| 1:D:517:THR:HG22 | 1:D:521:MSE:HE2  | 1.74                     | 0.70              |
| 1:G:319:GLU:O    | 1:G:323:MSE:HE3  | 1.90                     | 0.70              |
| 3:L:160:ASP:CB   | 3:L:282:LEU:HD11 | 2.22                     | 0.70              |
| 2:K:147:ILE:O    | 2:K:147:ILE:HD12 | 1.92                     | 0.69              |
| 1:A:346:ALA:HB1  | 1:A:384:ILE:HG12 | 1.72                     | 0.69              |
| 3:L:177:LEU:HD23 | 3:L:180:ILE:HD13 | 1.73                     | 0.69              |
| 3:L:272:GLN:OE1  | 3:L:288:GLN:NE2  | 2.25                     | 0.69              |
| 1:G:498:ARG:HG2  | 1:G:528:MSE:HE1  | 1.75                     | 0.69              |
| 1:J:69:LEU:HG    | 1:J:96:LEU:HD11  | 1.74                     | 0.69              |
| 3:I:237:VAL:HB   | 3:I:256:VAL:HG12 | 1.74                     | 0.69              |
| 3:L:276:MET:HE2  | 3:L:286:PHE:HE1  | 1.58                     | 0.68              |
| 3:I:48:VAL:HB    | 3:I:159:VAL:HG12 | 1.73                     | 0.68              |
| 1:D:245:MSE:HE1  | 1:D:248:LEU:HD23 | 1.76                     | 0.68              |
| 1:G:308:GLU:O    | 1:G:312:ASN:ND2  | 2.27                     | 0.68              |
| 1:D:22:ASN:O     | 1:D:28:ARG:NH1   | 2.27                     | 0.68              |
| 1:G:93:LEU:HB3   | 1:G:112:LEU:HD11 | 1.75                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:147:ILE:O    | 2:K:147:ILE:CD1  | 2.43                     | 0.67              |
| 1:A:505:ILE:HG23 | 1:A:521:MSE:HE3  | 1.76                     | 0.67              |
| 1:G:293:ASP:OD1  | 1:G:294:CYS:N    | 2.27                     | 0.67              |
| 2:H:25:THR:OG1   | 2:H:26:HIS:N     | 2.24                     | 0.67              |
| 2:E:149:PHE:CZ   | 2:E:151:GLU:HB2  | 2.29                     | 0.67              |
| 1:G:405:LEU:HG   | 1:G:438:PHE:HZ   | 1.59                     | 0.66              |
| 1:D:498:ARG:NH2  | 3:F:280:ASP:OD2  | 2.27                     | 0.66              |
| 1:D:100:GLU:HG3  | 2:E:25:THR:HG23  | 1.78                     | 0.66              |
| 3:I:239:ARG:HH21 | 3:I:241:HIS:HB3  | 1.61                     | 0.66              |
| 2:K:66:GLU:HG3   | 2:K:121:LEU:HD11 | 1.77                     | 0.65              |
| 1:G:144:ARG:NH2  | 1:G:178:THR:OG1  | 2.30                     | 0.65              |
| 1:J:381:ARG:NH1  | 1:J:410:GLU:OE1  | 2.29                     | 0.65              |
| 2:E:136:ILE:HD13 | 2:E:138:THR:HG23 | 1.79                     | 0.64              |
| 3:C:17:LEU:HD21  | 3:C:23:LEU:HD23  | 1.78                     | 0.64              |
| 2:E:174:VAL:HG23 | 2:E:179:PHE:HB3  | 1.79                     | 0.64              |
| 1:G:454:HIS:HB3  | 3:I:287:LEU:HD11 | 1.79                     | 0.64              |
| 1:J:538:PHE:HB3  | 1:J:575:VAL:HG22 | 1.79                     | 0.64              |
| 1:J:494:ASN:ND2  | 3:L:279:ASP:OD1  | 2.31                     | 0.64              |
| 3:C:202:ASP:HA   | 3:C:239:ARG:HH21 | 1.63                     | 0.64              |
| 1:D:32:ILE:O     | 1:D:72:GLN:NE2   | 2.31                     | 0.64              |
| 3:I:203:PRO:CD   | 3:I:239:ARG:NH1  | 2.61                     | 0.63              |
| 1:G:262:MSE:HE1  | 1:G:266:LYS:HD2  | 1.79                     | 0.63              |
| 2:E:195:ARG:HG2  | 2:E:218:GLU:HG3  | 1.80                     | 0.63              |
| 2:E:173:ARG:NH1  | 3:F:308:PHE:O    | 2.31                     | 0.63              |
| 1:G:108:ALA:O    | 1:G:112:LEU:HD13 | 1.98                     | 0.63              |
| 1:J:499:MSE:HE1  | 1:J:539:ASN:ND2  | 2.12                     | 0.63              |
| 1:G:176:ASP:OD1  | 1:G:177:ASP:N    | 2.30                     | 0.63              |
| 3:F:222:GLN:HE21 | 3:F:252:HIS:HA   | 1.63                     | 0.63              |
| 1:J:42:LEU:HG    | 1:J:46:ARG:HB2   | 1.81                     | 0.63              |
| 1:D:462:ALA:O    | 1:D:465:ASN:ND2  | 2.31                     | 0.63              |
| 3:F:264:ASN:HD22 | 3:F:267:TYR:HD1  | 1.45                     | 0.63              |
| 1:A:215:ASP:OD1  | 1:A:216:GLU:N    | 2.31                     | 0.63              |
| 3:C:152:TYR:O    | 3:C:185:ARG:NH2  | 2.32                     | 0.63              |
| 1:G:448:MSE:HE1  | 1:G:482:ILE:HA   | 1.80                     | 0.62              |
| 1:A:538:PHE:HB3  | 1:A:575:VAL:HG12 | 1.81                     | 0.62              |
| 1:D:588:LEU:HG   | 1:D:589:ALA:H    | 1.64                     | 0.62              |
| 1:J:55:LEU:HD23  | 1:J:69:LEU:HD11  | 1.82                     | 0.62              |
| 1:A:498:ARG:NH2  | 3:C:280:ASP:OD2  | 2.33                     | 0.62              |
| 2:B:184:ARG:NH1  | 2:B:236:ASN:OD1  | 2.31                     | 0.62              |
| 1:A:77:THR:OG1   | 1:A:118:GLU:OE2  | 2.18                     | 0.62              |
| 3:C:83:MET:HE2   | 3:C:240:ALA:HB2  | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:139:ASP:O    | 2:H:30:SER:N     | 2.32                     | 0.61              |
| 1:D:505:ILE:HG23 | 1:D:521:MSE:HE3  | 1.82                     | 0.61              |
| 1:A:459:ARG:O    | 1:A:463:THR:OG1  | 2.19                     | 0.61              |
| 1:D:381:ARG:NH1  | 1:D:410:GLU:OE1  | 2.33                     | 0.61              |
| 2:B:127:LEU:HD23 | 2:B:127:LEU:H    | 1.64                     | 0.61              |
| 1:D:583:LEU:HD23 | 1:D:589:ALA:C    | 2.26                     | 0.61              |
| 2:H:188:ARG:NH2  | 2:H:232:PHE:O    | 2.33                     | 0.61              |
| 1:A:171:ARG:HB2  | 1:A:208:MSE:HE2  | 1.82                     | 0.61              |
| 3:F:169:GLY:HA3  | 3:F:220:PHE:HZ   | 1.65                     | 0.60              |
| 1:D:462:ALA:C    | 1:D:465:ASN:ND2  | 2.59                     | 0.60              |
| 3:L:27:GLN:N     | 3:L:27:GLN:OE1   | 2.34                     | 0.60              |
| 1:J:459:ARG:NH1  | 1:J:496:LEU:O    | 2.34                     | 0.60              |
| 1:D:564:LEU:HB3  | 1:D:583:LEU:HD11 | 1.83                     | 0.60              |
| 1:J:356:LEU:HB3  | 1:J:360:ASN:HB2  | 1.83                     | 0.60              |
| 1:G:156:PRO:HG3  | 1:G:195:VAL:HG22 | 1.84                     | 0.60              |
| 3:L:54:VAL:HG23  | 3:L:259:ILE:HD13 | 1.84                     | 0.60              |
| 1:G:556:LEU:HA   | 1:G:560:VAL:HB   | 1.84                     | 0.60              |
| 1:A:414:ASP:OD1  | 1:A:415:ALA:N    | 2.34                     | 0.60              |
| 2:H:173:ARG:NH1  | 3:I:308:PHE:O    | 2.35                     | 0.60              |
| 3:F:244:VAL:HG21 | 3:F:249:ASN:HB2  | 1.84                     | 0.59              |
| 2:E:136:ILE:CD1  | 2:E:138:THR:HG23 | 2.33                     | 0.59              |
| 3:F:54:VAL:HG22  | 3:F:276:MET:HB3  | 1.84                     | 0.59              |
| 3:C:5:VAL:O      | 3:C:7:THR:N      | 2.35                     | 0.59              |
| 2:K:20:LEU:HD11  | 2:K:172:ILE:HD13 | 1.84                     | 0.59              |
| 1:G:222:LEU:HD12 | 1:G:258:ARG:HB3  | 1.84                     | 0.59              |
| 1:A:497:HIS:O    | 1:A:500:THR:OG1  | 2.19                     | 0.59              |
| 3:F:239:ARG:CZ   | 3:F:256:VAL:HG11 | 2.32                     | 0.59              |
| 1:G:420:ARG:NH1  | 1:G:453:ASP:OD2  | 2.36                     | 0.59              |
| 3:F:239:ARG:NH2  | 3:F:256:VAL:HG11 | 2.18                     | 0.58              |
| 1:J:45:GLU:N     | 1:J:45:GLU:OE1   | 2.35                     | 0.58              |
| 1:D:292:LYS:NZ   | 1:D:329:CYS:SG   | 2.77                     | 0.58              |
| 2:E:207:LYS:O    | 2:E:209:TYR:N    | 2.37                     | 0.58              |
| 3:F:83:MET:CE    | 3:F:238:SER:HB3  | 2.33                     | 0.58              |
| 1:G:338:ASN:O    | 1:G:341:VAL:HG12 | 2.03                     | 0.58              |
| 3:I:67:GLU:OE1   | 3:I:70:ARG:NH2   | 2.35                     | 0.58              |
| 3:C:10:LEU:HD12  | 3:C:106:ARG:HB2  | 1.86                     | 0.57              |
| 1:J:411:LEU:HB3  | 1:J:423:ILE:HG13 | 1.85                     | 0.57              |
| 1:A:572:ASP:O    | 1:A:575:VAL:HG22 | 2.04                     | 0.57              |
| 1:A:572:ASP:OD2  | 3:C:110:ARG:NH2  | 2.37                     | 0.57              |
| 2:E:183:LEU:HB3  | 2:E:199:THR:HB   | 1.86                     | 0.57              |
| 2:E:181:LEU:HB3  | 2:E:201:LEU:HB3  | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:50:CYS:HB2   | 3:L:51:PRO:HD3   | 1.87                     | 0.57              |
| 3:C:163:ILE:HG12 | 3:C:236:LEU:HD23 | 1.85                     | 0.57              |
| 1:G:32:ILE:HD12  | 1:G:65:VAL:HG13  | 1.87                     | 0.57              |
| 3:F:203:PRO:HG3  | 3:F:239:ARG:HH21 | 1.70                     | 0.57              |
| 3:C:10:LEU:CD1   | 3:C:106:ARG:HB2  | 2.35                     | 0.56              |
| 1:D:11:TYR:CE2   | 1:D:13:ILE:HG22  | 2.40                     | 0.56              |
| 3:F:139:ASN:ND2  | 3:F:141:ASN:OD1  | 2.35                     | 0.56              |
| 1:J:156:PRO:HG3  | 1:J:195:VAL:CG2  | 2.36                     | 0.56              |
| 1:G:260:ARG:NE   | 1:G:293:ASP:OD2  | 2.38                     | 0.56              |
| 1:J:551:LEU:O    | 1:J:552:ASP:OD1  | 2.24                     | 0.56              |
| 1:A:222:LEU:HD23 | 1:A:258:ARG:HB3  | 1.86                     | 0.56              |
| 1:D:206:ILE:HG22 | 1:D:207:PRO:HD3  | 1.87                     | 0.56              |
| 1:J:439:PHE:CE1  | 1:J:443:LEU:HD12 | 2.40                     | 0.56              |
| 1:J:67:LEU:HD11  | 1:J:103:VAL:HG22 | 1.88                     | 0.56              |
| 1:J:349:ILE:HD12 | 1:J:352:LEU:HD22 | 1.87                     | 0.56              |
| 1:D:318:ARG:HH21 | 1:D:355:ILE:HG12 | 1.69                     | 0.56              |
| 3:L:232:ASN:HB2  | 3:L:234:LEU:HD23 | 1.87                     | 0.56              |
| 1:A:37:THR:HA    | 1:A:40:LEU:HD23  | 1.88                     | 0.56              |
| 3:F:61:GLN:HE22  | 3:F:265:TYR:HA   | 1.70                     | 0.56              |
| 1:G:572:ASP:OD1  | 1:G:574:ASP:N    | 2.39                     | 0.56              |
| 2:B:150:PHE:HE1  | 2:B:171:LYS:HB2  | 1.70                     | 0.55              |
| 1:G:213:ALA:C    | 1:G:221:ARG:HG2  | 2.31                     | 0.55              |
| 2:B:127:LEU:HD12 | 2:B:252:LEU:HB3  | 1.87                     | 0.55              |
| 1:G:535:ASN:ND2  | 3:I:79:ASN:OD1   | 2.40                     | 0.55              |
| 3:F:6:PHE:HE1    | 3:F:9:GLU:HG2    | 1.71                     | 0.55              |
| 1:J:291:MSE:HG2  | 1:J:333:LEU:HD11 | 1.87                     | 0.55              |
| 3:I:10:LEU:HD23  | 3:I:106:ARG:HB2  | 1.89                     | 0.55              |
| 1:A:265:ASP:O    | 1:A:305:LYS:NZ   | 2.40                     | 0.55              |
| 2:K:160:LEU:HD21 | 2:K:166:SER:HB3  | 1.89                     | 0.55              |
| 3:C:164:PHE:HB2  | 3:C:234:LEU:CD2  | 2.37                     | 0.54              |
| 1:D:295:GLU:O    | 1:D:298:VAL:HG22 | 2.07                     | 0.54              |
| 1:D:400:LEU:HD23 | 1:D:400:LEU:H    | 1.72                     | 0.54              |
| 2:E:115:ASP:OD1  | 2:E:115:ASP:N    | 2.40                     | 0.54              |
| 2:H:174:VAL:HG12 | 2:H:179:PHE:HB2  | 1.90                     | 0.54              |
| 1:J:499:MSE:HE3  | 1:J:536:VAL:HA   | 1.89                     | 0.54              |
| 3:I:264:ASN:N    | 3:I:271:ASN:OD1  | 2.40                     | 0.54              |
| 1:G:7:HIS:HB3    | 1:J:28:ARG:HH12  | 1.71                     | 0.54              |
| 1:J:514:GLN:NE2  | 1:J:552:ASP:O    | 2.41                     | 0.54              |
| 2:E:45:LEU:HD13  | 2:E:49:MET:HG3   | 1.89                     | 0.54              |
| 2:H:212:ARG:NH2  | 2:H:250:GLU:OE1  | 2.40                     | 0.54              |
| 2:K:158:ASP:OD1  | 2:K:159:GLU:N    | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:155:TYR:CZ   | 1:J:163:LYS:HG3  | 2.43                     | 0.54              |
| 2:B:173:ARG:NH2  | 3:C:308:PHE:O    | 2.41                     | 0.54              |
| 3:F:239:ARG:NH1  | 3:F:256:VAL:HG11 | 2.22                     | 0.54              |
| 1:J:141:PHE:CE1  | 1:J:180:MSE:HG3  | 2.42                     | 0.54              |
| 1:A:570:ASP:HB3  | 1:A:575:VAL:CG2  | 2.31                     | 0.54              |
| 1:G:262:MSE:HE3  | 1:G:262:MSE:O    | 2.08                     | 0.54              |
| 1:J:263:VAL:O    | 1:J:267:PHE:N    | 2.41                     | 0.54              |
| 1:D:579:ALA:O    | 1:D:583:LEU:HD13 | 2.07                     | 0.54              |
| 1:J:495:TYR:CE1  | 3:L:51:PRO:HB2   | 2.43                     | 0.54              |
| 1:A:61:ASP:OD1   | 1:A:62:GLU:N     | 2.41                     | 0.53              |
| 1:A:517:THR:HG22 | 1:A:521:MSE:HE2  | 1.89                     | 0.53              |
| 1:J:495:TYR:HE1  | 3:L:51:PRO:HB2   | 1.73                     | 0.53              |
| 1:D:462:ALA:CA   | 1:D:465:ASN:ND2  | 2.72                     | 0.53              |
| 3:F:55:CYS:SG    | 3:F:275:ILE:HD11 | 2.48                     | 0.53              |
| 1:A:420:ARG:O    | 1:A:424:ILE:HG13 | 2.09                     | 0.53              |
| 1:A:502:LEU:HD23 | 1:A:539:ASN:HB3  | 1.91                     | 0.53              |
| 2:E:148:LYS:HB2  | 2:E:174:VAL:HG13 | 1.89                     | 0.53              |
| 1:G:205:ILE:HA   | 1:G:208:MSE:HE2  | 1.89                     | 0.53              |
| 3:L:241:HIS:O    | 3:L:241:HIS:ND1  | 2.41                     | 0.53              |
| 2:B:120:LEU:HD12 | 2:B:120:LEU:O    | 2.09                     | 0.53              |
| 1:D:272:LYS:HE3  | 1:D:312:ASN:OD1  | 2.09                     | 0.53              |
| 1:J:411:LEU:CB   | 1:J:423:ILE:HG13 | 2.39                     | 0.53              |
| 1:D:307:LYS:HB2  | 1:D:348:VAL:HB   | 1.90                     | 0.53              |
| 3:F:220:PHE:HE2  | 3:F:239:ARG:CZ   | 2.22                     | 0.53              |
| 1:J:35:LEU:HD11  | 1:J:55:LEU:HD21  | 1.90                     | 0.53              |
| 2:B:26:HIS:ND1   | 2:B:27:ILE:O     | 2.42                     | 0.53              |
| 1:G:489:MSE:HE2  | 1:G:501:THR:HB   | 1.91                     | 0.53              |
| 3:F:203:PRO:HB3  | 3:F:239:ARG:NH2  | 2.24                     | 0.53              |
| 2:B:168:LEU:HD11 | 2:B:183:LEU:HD11 | 1.91                     | 0.52              |
| 1:J:299:ARG:HE   | 1:J:341:VAL:HG11 | 1.74                     | 0.52              |
| 1:A:397:ILE:O    | 1:A:400:LEU:HD23 | 2.09                     | 0.52              |
| 3:C:5:VAL:HB     | 3:C:8:LYS:HE3    | 1.90                     | 0.52              |
| 2:E:76:VAL:HG12  | 2:E:77:ASN:H     | 1.75                     | 0.52              |
| 1:G:288:GLN:NE2  | 1:G:325:GLN:O    | 2.34                     | 0.52              |
| 1:G:299:ARG:NE   | 1:G:336:ASP:OD2  | 2.40                     | 0.52              |
| 2:H:17:PRO:O     | 2:H:60:GLY:N     | 2.43                     | 0.52              |
| 1:A:29:LEU:O     | 1:A:32:ILE:HG22  | 2.09                     | 0.52              |
| 1:G:156:PRO:HG3  | 1:G:195:VAL:CG2  | 2.40                     | 0.52              |
| 1:J:428:PRO:HD3  | 1:J:465:ASN:HD22 | 1.74                     | 0.52              |
| 2:K:25:THR:OG1   | 2:K:26:HIS:N     | 2.36                     | 0.52              |
| 1:A:192:PHE:O    | 1:A:195:VAL:HG12 | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:274:VAL:HB   | 1:G:278:ILE:HD11 | 1.90                     | 0.52              |
| 3:L:45:VAL:HG22  | 3:L:181:ARG:HG2  | 1.91                     | 0.52              |
| 3:F:121:ARG:HG3  | 3:F:147:THR:OG1  | 2.09                     | 0.52              |
| 3:C:203:PRO:CD   | 3:C:239:ARG:HE   | 2.23                     | 0.52              |
| 2:E:50:PHE:HB3   | 2:E:53:ASN:OD1   | 2.10                     | 0.52              |
| 2:H:207:LYS:O    | 2:H:209:TYR:N    | 2.42                     | 0.52              |
| 3:I:17:LEU:HD21  | 3:I:98:THR:HG22  | 1.91                     | 0.52              |
| 2:K:64:GLY:O     | 2:K:121:LEU:N    | 2.39                     | 0.52              |
| 2:B:207:LYS:O    | 2:B:209:TYR:N    | 2.43                     | 0.52              |
| 1:D:405:LEU:HG   | 1:D:406:PRO:HD3  | 1.91                     | 0.52              |
| 3:F:99:LEU:O     | 3:F:103:LEU:HD12 | 2.10                     | 0.52              |
| 3:I:88:ASP:OD2   | 3:I:118:HIS:HB3  | 2.09                     | 0.52              |
| 2:K:123:GLU:N    | 2:K:123:GLU:OE1  | 2.42                     | 0.52              |
| 1:A:35:LEU:O     | 1:A:38:ILE:HG22  | 2.09                     | 0.52              |
| 3:F:85:ASP:OD1   | 3:F:167:HIS:CE1  | 2.62                     | 0.52              |
| 1:G:56:THR:HA    | 1:G:92:PRO:HA    | 1.92                     | 0.52              |
| 1:J:19:GLU:OE2   | 1:J:31:SER:OG    | 2.27                     | 0.52              |
| 2:H:149:PHE:CD2  | 1:J:6:SER:HB2    | 2.46                     | 0.51              |
| 1:J:28:ARG:NH1   | 1:J:62:GLU:OE2   | 2.44                     | 0.51              |
| 2:K:219:SER:HB2  | 2:K:243:PRO:HD2  | 1.91                     | 0.51              |
| 3:F:121:ARG:N    | 3:F:188:GLU:OE1  | 2.43                     | 0.51              |
| 3:L:49:ARG:NH1   | 3:L:110:ARG:NH2  | 2.56                     | 0.51              |
| 3:L:276:MET:HA   | 3:L:285:SER:O    | 2.11                     | 0.51              |
| 1:D:334:VAL:HG21 | 1:D:368:LEU:HD12 | 1.93                     | 0.51              |
| 1:G:155:TYR:OH   | 1:G:167:ARG:NH1  | 2.42                     | 0.51              |
| 1:G:354:PRO:HD3  | 1:G:390:CYS:SG   | 2.50                     | 0.51              |
| 1:G:531:ASP:O    | 1:G:537:ARG:NH1  | 2.44                     | 0.51              |
| 3:C:76:PRO:HB2   | 3:C:110:ARG:HG3  | 1.92                     | 0.51              |
| 1:D:577:TYR:O    | 1:D:581:GLU:N    | 2.39                     | 0.51              |
| 1:G:48:ARG:HA    | 1:G:52:LEU:HD13  | 1.92                     | 0.51              |
| 3:I:121:ARG:N    | 3:I:188:GLU:OE2  | 2.44                     | 0.51              |
| 3:L:107:TYR:HB3  | 3:L:110:ARG:HB2  | 1.92                     | 0.51              |
| 1:G:544:LEU:HD23 | 1:G:560:VAL:HG13 | 1.93                     | 0.51              |
| 3:I:17:LEU:HD22  | 3:I:99:LEU:HA    | 1.92                     | 0.51              |
| 3:F:6:PHE:O      | 3:F:8:LYS:N      | 2.43                     | 0.51              |
| 2:H:114:THR:HG22 | 2:H:116:TYR:H    | 1.76                     | 0.51              |
| 3:L:110:ARG:HG2  | 3:L:110:ARG:HH11 | 1.76                     | 0.51              |
| 1:A:124:LEU:HD22 | 1:A:128:PHE:HB3  | 1.93                     | 0.50              |
| 1:A:156:PRO:HB2  | 3:F:231:ALA:HA   | 1.92                     | 0.50              |
| 1:D:409:VAL:O    | 1:D:413:GLU:HG2  | 2.11                     | 0.50              |
| 1:J:350:MSE:SE   | 1:J:391:VAL:HG21 | 2.61                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:ARG:NH1  | 1:A:149:GLY:O    | 2.40                     | 0.50              |
| 1:A:254:ASP:O    | 1:A:260:ARG:NH1  | 2.40                     | 0.50              |
| 1:D:229:VAL:O    | 1:D:233:GLN:HG3  | 2.11                     | 0.50              |
| 3:L:110:ARG:HG2  | 3:L:110:ARG:NH1  | 2.26                     | 0.50              |
| 2:E:55:LEU:HD23  | 2:E:170:VAL:HG23 | 1.93                     | 0.50              |
| 3:L:81:LEU:HD22  | 3:L:112:THR:HB   | 1.92                     | 0.50              |
| 3:L:156:THR:HG22 | 3:L:166:LEU:CB   | 2.39                     | 0.50              |
| 2:B:20:LEU:HG    | 2:B:57:ILE:HG22  | 1.92                     | 0.50              |
| 2:E:172:ILE:HD12 | 2:E:181:LEU:HD12 | 1.92                     | 0.50              |
| 1:G:88:CYS:O     | 1:G:91:PRO:HD2   | 2.12                     | 0.50              |
| 3:I:279:ASP:OD1  | 3:I:283:LYS:N    | 2.45                     | 0.50              |
| 1:G:357:GLY:O    | 1:G:361:THR:HG23 | 2.12                     | 0.50              |
| 2:H:198:ASP:HB2  | 2:H:215:THR:HG23 | 1.94                     | 0.50              |
| 3:L:132:GLU:HG2  | 3:L:135:ARG:HH21 | 1.77                     | 0.50              |
| 3:L:250:TRP:CE3  | 3:L:254:ARG:HG3  | 2.47                     | 0.50              |
| 1:A:76:PHE:HB3   | 1:A:89:LEU:HD11  | 1.94                     | 0.50              |
| 3:C:121:ARG:HG2  | 3:C:147:THR:HB   | 1.94                     | 0.50              |
| 1:D:215:ASP:OD1  | 1:D:216:GLU:N    | 2.45                     | 0.50              |
| 3:F:203:PRO:CG   | 3:F:239:ARG:HH21 | 2.25                     | 0.50              |
| 2:B:37:ALA:O     | 2:B:42:MET:N     | 2.45                     | 0.49              |
| 3:F:87:VAL:O     | 3:F:93:SER:OG    | 2.24                     | 0.49              |
| 1:G:25:VAL:HA    | 1:G:28:ARG:HD3   | 1.94                     | 0.49              |
| 1:J:291:MSE:HE1  | 1:J:330:ILE:HG22 | 1.93                     | 0.49              |
| 1:J:505:ILE:HG21 | 1:J:525:VAL:HG21 | 1.94                     | 0.49              |
| 2:E:149:PHE:CE1  | 2:E:151:GLU:HB2  | 2.48                     | 0.49              |
| 2:H:188:ARG:NH2  | 2:H:233:THR:HA   | 2.27                     | 0.49              |
| 2:K:55:LEU:HD12  | 2:K:55:LEU:O     | 2.12                     | 0.49              |
| 1:D:222:LEU:HD12 | 1:D:262:MSE:HE2  | 1.95                     | 0.49              |
| 1:D:448:MSE:HE2  | 1:D:448:MSE:HA   | 1.94                     | 0.49              |
| 1:A:279:THR:HA   | 1:A:283:LEU:HB2  | 1.94                     | 0.49              |
| 1:D:294:CYS:O    | 1:D:299:ARG:NH1  | 2.44                     | 0.49              |
| 3:F:85:ASP:OD1   | 3:F:167:HIS:NE2  | 2.46                     | 0.49              |
| 3:L:246:GLU:O    | 3:L:248:TYR:N    | 2.46                     | 0.49              |
| 1:A:194:LYS:HA   | 1:A:234:LEU:HD21 | 1.95                     | 0.49              |
| 1:A:271:GLN:HA   | 1:A:274:VAL:HG12 | 1.94                     | 0.49              |
| 3:L:84:GLY:HA2   | 3:L:86:TYR:CZ    | 2.48                     | 0.49              |
| 1:J:194:LYS:HA   | 1:J:234:LEU:HD11 | 1.95                     | 0.49              |
| 1:J:487:LEU:HD11 | 1:J:524:THR:HG21 | 1.95                     | 0.49              |
| 2:K:166:SER:HB2  | 2:K:187:LEU:HD23 | 1.95                     | 0.49              |
| 3:C:125:GLN:HA   | 3:C:130:TYR:HB3  | 1.95                     | 0.49              |
| 1:D:456:TYR:CD2  | 3:F:73:GLY:HA2   | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:164:GLY:O    | 2:E:165:VAL:HG23 | 2.12                     | 0.49              |
| 1:J:326:ILE:O    | 1:J:330:ILE:HG23 | 2.13                     | 0.49              |
| 1:J:529:ALA:HB1  | 1:J:567:LEU:HD21 | 1.95                     | 0.49              |
| 2:B:56:ARG:NH2   | 2:B:66:GLU:OE1   | 2.43                     | 0.49              |
| 3:I:251:CYS:SG   | 3:I:256:VAL:HG23 | 2.52                     | 0.49              |
| 1:A:414:ASP:O    | 1:A:420:ARG:HD2  | 2.13                     | 0.48              |
| 1:A:548:GLY:HA2  | 1:A:551:LEU:HD21 | 1.95                     | 0.48              |
| 3:C:50:CYS:HB2   | 3:C:51:PRO:HD3   | 1.94                     | 0.48              |
| 1:J:522:LEU:HD22 | 1:J:551:LEU:HD11 | 1.93                     | 0.48              |
| 3:C:126:VAL:HG13 | 3:C:127:TYR:CD1  | 2.48                     | 0.48              |
| 1:D:11:TYR:O     | 1:D:14:ALA:N     | 2.43                     | 0.48              |
| 3:I:85:ASP:CG    | 3:I:167:HIS:CE1  | 2.91                     | 0.48              |
| 1:D:245:MSE:HA   | 1:D:245:MSE:HE2  | 1.95                     | 0.48              |
| 1:G:350:MSE:HG3  | 1:G:391:VAL:CG2  | 2.42                     | 0.48              |
| 1:G:409:VAL:O    | 1:G:413:GLU:HG2  | 2.13                     | 0.48              |
| 3:L:47:GLU:HG2   | 3:L:158:LEU:HB3  | 1.96                     | 0.48              |
| 2:B:13:PHE:HB3   | 2:B:20:LEU:HB3   | 1.94                     | 0.48              |
| 1:D:537:ARG:NH2  | 1:D:570:ASP:OD2  | 2.42                     | 0.48              |
| 1:J:495:TYR:O    | 1:J:498:ARG:N    | 2.47                     | 0.48              |
| 1:A:535:ASN:HA   | 1:A:538:PHE:CE2  | 2.49                     | 0.48              |
| 1:G:385:ILE:HA   | 1:G:388:LEU:HD21 | 1.95                     | 0.48              |
| 3:I:44:ASN:HD22  | 3:I:185:ARG:HD3  | 1.79                     | 0.48              |
| 1:J:295:GLU:HG3  | 1:J:296:ALA:H    | 1.78                     | 0.48              |
| 2:K:69:ALA:HB2   | 2:K:155:LEU:HB3  | 1.94                     | 0.48              |
| 1:A:40:LEU:HD13  | 1:A:79:LEU:HD11  | 1.96                     | 0.48              |
| 1:D:535:ASN:O    | 1:D:539:ASN:ND2  | 2.39                     | 0.48              |
| 1:J:510:GLU:HG3  | 1:J:511:VAL:HG22 | 1.96                     | 0.48              |
| 2:K:28:MET:HG3   | 2:K:33:VAL:HG22  | 1.95                     | 0.48              |
| 2:E:149:PHE:CD1  | 2:E:150:PHE:N    | 2.82                     | 0.48              |
| 3:F:59:HIS:NE2   | 3:F:85:ASP:OD2   | 2.47                     | 0.48              |
| 1:A:280:LYS:HD2  | 1:A:317:CYS:SG   | 2.54                     | 0.48              |
| 2:K:221:ILE:HD12 | 2:K:222:ALA:N    | 2.28                     | 0.48              |
| 3:F:275:ILE:HG22 | 3:F:287:LEU:HB2  | 1.96                     | 0.47              |
| 1:J:124:LEU:HD22 | 1:J:128:PHE:HB3  | 1.94                     | 0.47              |
| 1:J:416:LYS:HG3  | 1:J:419:VAL:HG12 | 1.94                     | 0.47              |
| 2:K:45:LEU:HB2   | 2:K:46:PRO:HD2   | 1.94                     | 0.47              |
| 3:L:57:ASP:HB2   | 3:L:260:PHE:CE1  | 2.49                     | 0.47              |
| 1:D:287:PHE:HD2  | 1:D:326:ILE:HD11 | 1.79                     | 0.47              |
| 1:D:418:ARG:NH2  | 3:F:67:GLU:OE1   | 2.46                     | 0.47              |
| 1:G:52:LEU:O     | 1:G:56:THR:HG23  | 2.14                     | 0.47              |
| 3:I:29:LYS:O     | 3:I:33:GLU:HG2   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:71:ILE:CG2   | 3:I:287:LEU:HD23 | 2.44                     | 0.47              |
| 1:J:174:CYS:SG   | 1:J:208:MSE:HE3  | 2.55                     | 0.47              |
| 1:D:564:LEU:HD13 | 1:D:583:LEU:HD11 | 1.97                     | 0.47              |
| 2:E:45:LEU:HB2   | 2:E:46:PRO:HD2   | 1.96                     | 0.47              |
| 2:E:149:PHE:H    | 2:E:174:VAL:HG12 | 1.79                     | 0.47              |
| 1:J:391:VAL:O    | 1:J:395:ILE:HG23 | 2.14                     | 0.47              |
| 1:G:22:ASN:O     | 1:G:28:ARG:HD2   | 2.14                     | 0.47              |
| 1:D:11:TYR:CD2   | 1:D:13:ILE:HG22  | 2.49                     | 0.47              |
| 1:D:52:LEU:O     | 1:D:56:THR:HG23  | 2.14                     | 0.47              |
| 1:G:493:PRO:O    | 1:G:498:ARG:NH1  | 2.47                     | 0.47              |
| 1:A:524:THR:O    | 1:A:528:MSE:HG3  | 2.14                     | 0.47              |
| 1:D:245:MSE:SE   | 1:D:278:ILE:HG21 | 2.65                     | 0.47              |
| 1:A:222:LEU:HD12 | 1:A:223:LEU:N    | 2.30                     | 0.47              |
| 3:C:126:VAL:HG13 | 3:C:127:TYR:HD1  | 1.78                     | 0.47              |
| 1:G:346:ALA:HB2  | 1:G:380:VAL:HG23 | 1.96                     | 0.47              |
| 2:H:149:PHE:CE2  | 1:J:6:SER:HB2    | 2.50                     | 0.47              |
| 3:I:252:HIS:O    | 3:I:255:ASN:ND2  | 2.43                     | 0.47              |
| 1:J:552:ASP:HB3  | 1:J:555:THR:HG23 | 1.96                     | 0.47              |
| 3:L:83:MET:O     | 3:L:167:HIS:ND1  | 2.45                     | 0.47              |
| 1:D:322:ILE:HA   | 1:D:326:ILE:HG22 | 1.97                     | 0.47              |
| 1:G:215:ASP:OD1  | 1:G:217:GLN:N    | 2.47                     | 0.47              |
| 3:L:304:THR:O    | 3:L:305:PRO:C    | 2.58                     | 0.47              |
| 1:D:465:ASN:HD22 | 1:D:465:ASN:H    | 1.63                     | 0.47              |
| 1:G:61:ASP:OD1   | 1:G:62:GLU:N     | 2.47                     | 0.47              |
| 2:H:204:GLU:HB3  | 2:H:207:LYS:HG3  | 1.96                     | 0.47              |
| 3:I:202:ASP:OD1  | 3:I:239:ARG:NH2  | 2.47                     | 0.47              |
| 1:J:219:SER:O    | 1:J:222:LEU:HD23 | 2.15                     | 0.47              |
| 1:D:29:LEU:HD22  | 1:D:33:LYS:HE2   | 1.97                     | 0.47              |
| 1:D:323:MSE:HE1  | 1:D:360:ASN:CG   | 2.39                     | 0.47              |
| 1:J:391:VAL:O    | 1:J:391:VAL:HG12 | 2.14                     | 0.47              |
| 1:G:97:ALA:HA    | 1:G:105:ARG:HA   | 1.96                     | 0.46              |
| 1:J:90:LEU:HB2   | 1:J:91:PRO:HD3   | 1.96                     | 0.46              |
| 1:J:170:PHE:CD2  | 1:J:208:MSE:HE1  | 2.50                     | 0.46              |
| 1:D:76:PHE:O     | 1:D:80:VAL:N     | 2.46                     | 0.46              |
| 3:F:263:PRO:HB2  | 3:F:291:PRO:HD3  | 1.97                     | 0.46              |
| 1:G:21:ARG:HH22  | 1:J:8:MSE:N      | 2.13                     | 0.46              |
| 1:A:547:ILE:O    | 1:A:551:LEU:HD23 | 2.15                     | 0.46              |
| 1:D:572:ASP:OD1  | 3:F:110:ARG:NH2  | 2.49                     | 0.46              |
| 1:G:7:HIS:CD2    | 1:J:28:ARG:HH22  | 2.33                     | 0.46              |
| 1:J:138:GLY:O    | 1:J:144:ARG:NH1  | 2.49                     | 0.46              |
| 1:D:322:ILE:HA   | 1:D:326:ILE:CG2  | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:170:LEU:HD12 | 3:I:220:PHE:CZ   | 2.51                     | 0.46              |
| 3:L:58:VAL:HG21  | 3:L:65:LEU:HD12  | 1.98                     | 0.46              |
| 1:A:311:GLU:O    | 1:A:318:ARG:NH1  | 2.49                     | 0.46              |
| 1:D:538:PHE:HB3  | 1:D:575:VAL:HA   | 1.97                     | 0.46              |
| 1:G:93:LEU:HD13  | 1:G:112:LEU:HD12 | 1.96                     | 0.46              |
| 2:H:109:ASP:OD1  | 2:H:111:THR:N    | 2.43                     | 0.46              |
| 3:I:239:ARG:HD3  | 3:I:239:ARG:C    | 2.41                     | 0.46              |
| 2:B:198:ASP:N    | 2:B:215:THR:O    | 2.48                     | 0.46              |
| 3:L:57:ASP:OD2   | 3:L:241:HIS:HA   | 2.16                     | 0.46              |
| 1:D:11:TYR:CD1   | 1:D:12:PRO:HD2   | 2.51                     | 0.46              |
| 3:F:83:MET:HE3   | 3:F:238:SER:HB3  | 1.97                     | 0.46              |
| 3:F:50:CYS:HB3   | 3:F:160:ASP:HB2  | 1.98                     | 0.46              |
| 3:F:252:HIS:O    | 3:F:255:ASN:ND2  | 2.43                     | 0.46              |
| 1:G:300:ALA:HA   | 1:G:341:VAL:HG23 | 1.98                     | 0.46              |
| 1:A:79:LEU:HD13  | 1:D:532:PRO:HG3  | 1.98                     | 0.46              |
| 1:D:156:PRO:HG3  | 1:D:195:VAL:HG13 | 1.98                     | 0.46              |
| 1:J:144:ARG:NE   | 1:J:176:ASP:OD2  | 2.49                     | 0.46              |
| 2:K:66:GLU:N     | 2:K:119:THR:O    | 2.46                     | 0.46              |
| 3:L:97:VAL:O     | 3:L:101:VAL:HG23 | 2.16                     | 0.46              |
| 1:G:525:VAL:HG12 | 1:G:544:LEU:HD11 | 1.97                     | 0.46              |
| 1:G:538:PHE:HB3  | 1:G:575:VAL:HA   | 1.98                     | 0.46              |
| 1:J:357:GLY:O    | 1:J:361:THR:N    | 2.44                     | 0.46              |
| 1:A:404:LEU:HD23 | 1:A:404:LEU:H    | 1.81                     | 0.45              |
| 3:C:23:LEU:HD12  | 3:C:27:GLN:HB3   | 1.97                     | 0.45              |
| 3:I:67:GLU:O     | 3:I:71:ILE:HD12  | 2.16                     | 0.45              |
| 1:J:11:TYR:HD1   | 1:J:12:PRO:HD2   | 1.81                     | 0.45              |
| 2:K:173:ARG:NH2  | 3:L:308:PHE:O    | 2.49                     | 0.45              |
| 3:C:252:HIS:O    | 3:C:255:ASN:HB2  | 2.16                     | 0.45              |
| 1:G:7:HIS:CG     | 1:J:28:ARG:HH22  | 2.34                     | 0.45              |
| 1:G:109:VAL:HA   | 1:G:112:LEU:HD22 | 1.98                     | 0.45              |
| 1:G:353:SER:N    | 1:G:354:PRO:HD2  | 2.31                     | 0.45              |
| 2:H:187:LEU:HB3  | 2:H:195:ARG:HB3  | 1.97                     | 0.45              |
| 1:A:12:PRO:O     | 1:A:15:VAL:HG12  | 2.16                     | 0.45              |
| 1:A:156:PRO:HG3  | 1:A:195:VAL:HG22 | 1.97                     | 0.45              |
| 1:D:554:SER:O    | 1:D:558:SER:OG   | 2.27                     | 0.45              |
| 3:F:45:VAL:HG12  | 3:F:156:THR:OG1  | 2.16                     | 0.45              |
| 3:F:95:GLU:OE1   | 3:F:95:GLU:N     | 2.40                     | 0.45              |
| 1:G:375:ASP:OD1  | 1:G:376:GLU:N    | 2.48                     | 0.45              |
| 3:I:54:VAL:HG22  | 3:I:83:MET:HE2   | 1.98                     | 0.45              |
| 1:J:180:MSE:H    | 1:J:180:MSE:SE   | 2.50                     | 0.45              |
| 2:H:44:SER:O     | 2:H:45:LEU:HD12  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:436:VAL:HG13 | 1:J:437:GLU:H    | 1.81                     | 0.45              |
| 2:B:172:ILE:HB   | 2:B:181:LEU:HD12 | 1.99                     | 0.45              |
| 3:C:115:ARG:HG2  | 3:C:119:GLU:HB2  | 1.99                     | 0.45              |
| 1:G:201:VAL:HG13 | 1:G:205:ILE:HG21 | 1.99                     | 0.45              |
| 3:I:17:LEU:HD22  | 3:I:99:LEU:CA    | 2.47                     | 0.45              |
| 1:J:467:LYS:HD2  | 1:J:510:GLU:OE2  | 2.16                     | 0.45              |
| 2:K:33:VAL:HG12  | 2:K:45:LEU:HD21  | 1.99                     | 0.45              |
| 1:A:144:ARG:HB3  | 1:A:181:VAL:HG11 | 1.97                     | 0.45              |
| 3:F:237:VAL:O    | 3:F:256:VAL:HG13 | 2.16                     | 0.45              |
| 1:A:98:THR:HG22  | 1:A:143:SER:HB3  | 1.98                     | 0.45              |
| 3:C:160:ASP:HB3  | 3:C:282:LEU:HD11 | 1.99                     | 0.45              |
| 1:D:180:MSE:HE1  | 2:E:47:GLU:HB3   | 1.99                     | 0.45              |
| 1:J:156:PRO:HG3  | 1:J:195:VAL:HG21 | 1.99                     | 0.45              |
| 1:J:291:MSE:CE   | 1:J:330:ILE:HG22 | 2.47                     | 0.45              |
| 1:D:318:ARG:O    | 1:D:322:ILE:HG12 | 2.16                     | 0.45              |
| 3:F:237:VAL:HB   | 3:F:256:VAL:HG13 | 1.99                     | 0.45              |
| 1:G:319:GLU:HG2  | 1:G:323:MSE:HE1  | 1.99                     | 0.45              |
| 2:K:148:LYS:HB3  | 2:K:148:LYS:HE2  | 1.81                     | 0.45              |
| 1:A:115:ILE:O    | 1:A:119:HIS:ND1  | 2.45                     | 0.45              |
| 1:D:215:ASP:O    | 1:D:221:ARG:NH1  | 2.49                     | 0.45              |
| 1:G:387:ASN:C    | 1:G:388:LEU:HD23 | 2.41                     | 0.45              |
| 3:L:84:GLY:HA2   | 3:L:86:TYR:CE2   | 2.51                     | 0.45              |
| 3:F:115:ARG:NH1  | 3:F:119:GLU:O    | 2.49                     | 0.45              |
| 1:J:424:ILE:HG21 | 1:J:461:ALA:HB1  | 1.98                     | 0.45              |
| 1:D:8:MSE:HE2    | 1:D:8:MSE:HB2    | 1.82                     | 0.44              |
| 1:G:430:LEU:O    | 1:G:434:LEU:HB2  | 2.17                     | 0.44              |
| 2:K:203:HIS:HB2  | 2:K:210:MET:HB3  | 1.99                     | 0.44              |
| 1:D:105:ARG:O    | 1:D:109:VAL:HG23 | 2.17                     | 0.44              |
| 1:G:141:PHE:HB2  | 1:G:178:THR:HG21 | 1.99                     | 0.44              |
| 3:C:143:TRP:O    | 3:C:147:THR:OG1  | 2.28                     | 0.44              |
| 1:G:401:SER:O    | 1:G:405:LEU:HD12 | 2.18                     | 0.44              |
| 1:J:303:SER:HB3  | 1:J:345:LEU:HB2  | 1.98                     | 0.44              |
| 1:D:455:VAL:HG13 | 3:F:71:ILE:HG12  | 1.99                     | 0.44              |
| 3:F:256:VAL:HG12 | 3:F:257:VAL:N    | 2.33                     | 0.44              |
| 3:I:17:LEU:HD11  | 3:I:23:LEU:HD11  | 1.98                     | 0.44              |
| 3:I:244:VAL:HG22 | 3:I:246:GLU:H    | 1.82                     | 0.44              |
| 1:D:357:GLY:O    | 1:D:361:THR:OG1  | 2.33                     | 0.44              |
| 2:H:174:VAL:HG12 | 2:H:179:PHE:CB   | 2.48                     | 0.44              |
| 3:I:13:TRP:O     | 3:I:14:ILE:C     | 2.60                     | 0.44              |
| 3:I:159:VAL:HG22 | 3:I:163:ILE:HB   | 2.00                     | 0.44              |
| 1:J:583:LEU:HD13 | 1:J:583:LEU:O    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:260:PHE:CZ   | 3:L:262:ALA:HB3  | 2.52                     | 0.44              |
| 3:C:279:ASP:OD1  | 3:C:281:THR:O    | 2.35                     | 0.44              |
| 1:J:535:ASN:O    | 1:J:539:ASN:ND2  | 2.51                     | 0.44              |
| 3:L:73:GLY:O     | 3:L:80:TYR:OH    | 2.28                     | 0.44              |
| 1:A:198:LEU:O    | 1:A:201:VAL:HG12 | 2.18                     | 0.44              |
| 3:C:68:LEU:HD11  | 3:C:275:ILE:HG21 | 1.99                     | 0.44              |
| 1:D:459:ARG:NH2  | 1:D:496:LEU:HG   | 2.33                     | 0.44              |
| 1:J:180:MSE:HA   | 1:J:183:ARG:HG2  | 2.00                     | 0.44              |
| 2:K:50:PHE:HB3   | 2:K:53:ASN:HD21  | 1.83                     | 0.44              |
| 2:K:248:VAL:HG23 | 2:K:249:CYS:N    | 2.32                     | 0.44              |
| 3:L:286:PHE:O    | 3:L:287:LEU:HD12 | 2.17                     | 0.44              |
| 1:D:56:THR:HG22  | 1:D:92:PRO:HD3   | 1.99                     | 0.44              |
| 2:E:45:LEU:HB2   | 2:E:46:PRO:CD    | 2.48                     | 0.44              |
| 3:I:206:ARG:HH21 | 3:I:210:GLY:HA3  | 1.82                     | 0.44              |
| 1:J:42:LEU:HD12  | 1:J:46:ARG:HE    | 1.83                     | 0.44              |
| 1:J:303:SER:O    | 1:J:345:LEU:HD23 | 2.18                     | 0.44              |
| 3:L:48:VAL:HG22  | 3:L:49:ARG:HG2   | 2.00                     | 0.44              |
| 3:L:85:ASP:OD2   | 3:L:167:HIS:CE1  | 2.71                     | 0.44              |
| 1:A:350:MSE:HA   | 1:A:350:MSE:HE2  | 1.99                     | 0.44              |
| 2:B:109:ASP:OD1  | 2:B:111:THR:N    | 2.39                     | 0.44              |
| 3:F:175:ASP:O    | 3:F:232:ASN:ND2  | 2.48                     | 0.44              |
| 1:G:389:ASP:N    | 1:G:389:ASP:OD1  | 2.50                     | 0.44              |
| 1:J:180:MSE:HE1  | 2:K:47:GLU:OE1   | 2.18                     | 0.44              |
| 1:J:392:ASN:OD1  | 1:J:397:ILE:HG12 | 2.18                     | 0.44              |
| 1:J:410:GLU:O    | 1:J:414:ASP:N    | 2.51                     | 0.44              |
| 3:L:125:GLN:HA   | 3:L:130:TYR:HB3  | 2.00                     | 0.44              |
| 2:E:202:TYR:OH   | 2:E:204:GLU:HG3  | 2.18                     | 0.43              |
| 1:J:156:PRO:HG3  | 1:J:195:VAL:HG22 | 1.99                     | 0.43              |
| 1:J:317:CYS:HB2  | 1:J:321:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:427:MSE:O    | 1:A:431:ALA:N    | 2.48                     | 0.43              |
| 1:D:113:ARG:O    | 1:D:116:SER:OG   | 2.36                     | 0.43              |
| 3:F:119:GLU:OE1  | 3:F:119:GLU:N    | 2.50                     | 0.43              |
| 1:G:539:ASN:O    | 1:G:543:SER:N    | 2.51                     | 0.43              |
| 1:J:540:VAL:O    | 1:J:544:LEU:HD22 | 2.18                     | 0.43              |
| 3:L:290:ASP:OD1  | 3:L:290:ASP:N    | 2.51                     | 0.43              |
| 3:F:44:ASN:HD22  | 3:F:185:ARG:HD3  | 1.83                     | 0.43              |
| 1:D:197:GLU:N    | 1:D:197:GLU:OE1  | 2.51                     | 0.43              |
| 1:D:287:PHE:O    | 1:D:291:MSE:HG3  | 2.18                     | 0.43              |
| 1:G:194:LYS:HG3  | 1:G:195:VAL:N    | 2.34                     | 0.43              |
| 3:I:109:GLU:OE2  | 3:I:109:GLU:HA   | 2.18                     | 0.43              |
| 1:D:80:VAL:HG21  | 1:D:89:LEU:HD21  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:248:LEU:HD12 | 1:D:248:LEU:O    | 2.18                     | 0.43              |
| 3:I:39:LEU:HD13  | 3:I:153:LEU:HD23 | 2.00                     | 0.43              |
| 1:J:133:LYS:O    | 1:J:137:GLY:N    | 2.47                     | 0.43              |
| 1:J:416:LYS:HG3  | 1:J:419:VAL:CG1  | 2.49                     | 0.43              |
| 2:K:20:LEU:CD1   | 2:K:172:ILE:HD13 | 2.46                     | 0.43              |
| 3:F:261:SER:HA   | 3:F:273:ALA:HB1  | 2.01                     | 0.43              |
| 1:G:73:LEU:HA    | 1:G:76:PHE:HD2   | 1.84                     | 0.43              |
| 3:I:202:ASP:OD2  | 3:I:214:ARG:NH2  | 2.52                     | 0.43              |
| 1:A:112:LEU:HD23 | 1:A:115:ILE:HD11 | 2.01                     | 0.43              |
| 1:G:307:LYS:HB2  | 1:G:348:VAL:HB   | 2.00                     | 0.43              |
| 2:H:50:PHE:HB3   | 2:H:53:ASN:CG    | 2.44                     | 0.43              |
| 1:D:295:GLU:O    | 1:D:297:GLU:N    | 2.52                     | 0.43              |
| 3:F:49:ARG:HD2   | 3:F:49:ARG:HA    | 1.78                     | 0.43              |
| 1:G:140:TRP:CD1  | 1:G:140:TRP:N    | 2.86                     | 0.43              |
| 1:J:124:LEU:HD11 | 1:J:154:CYS:HB2  | 2.00                     | 0.43              |
| 1:J:478:ALA:O    | 1:J:482:ILE:HB   | 2.18                     | 0.43              |
| 1:A:156:PRO:CG   | 1:A:195:VAL:HG22 | 2.49                     | 0.43              |
| 1:A:499:MSE:HE3  | 1:A:539:ASN:ND2  | 2.34                     | 0.43              |
| 1:D:14:ALA:HA    | 1:D:17:ILE:HD12  | 2.00                     | 0.43              |
| 1:D:318:ARG:NH2  | 1:D:355:ILE:HG12 | 2.31                     | 0.43              |
| 2:E:170:VAL:HG11 | 2:E:183:LEU:HD12 | 2.01                     | 0.43              |
| 3:F:50:CYS:N     | 3:F:51:PRO:HD3   | 2.34                     | 0.43              |
| 2:B:141:LEU:HD12 | 2:B:141:LEU:H    | 1.83                     | 0.43              |
| 3:C:203:PRO:HD3  | 3:C:239:ARG:HE   | 1.84                     | 0.43              |
| 3:C:239:ARG:HH12 | 3:C:241:HIS:N    | 2.17                     | 0.43              |
| 1:D:439:PHE:CZ   | 1:D:469:LEU:HD21 | 2.53                     | 0.43              |
| 3:I:290:ASP:HB3  | 3:I:291:PRO:HD2  | 2.01                     | 0.43              |
| 2:K:113:THR:CG2  | 2:K:195:ARG:HH12 | 2.32                     | 0.43              |
| 2:K:200:ARG:NH2  | 3:L:309:LEU:O    | 2.51                     | 0.43              |
| 2:K:219:SER:OG   | 2:K:223:ASN:ND2  | 2.51                     | 0.43              |
| 1:A:180:MSE:HE2  | 2:B:48:MET:HE2   | 2.01                     | 0.42              |
| 1:A:183:ARG:HB3  | 1:A:223:LEU:HD12 | 2.00                     | 0.42              |
| 3:F:115:ARG:NH1  | 3:F:189:VAL:HG23 | 2.34                     | 0.42              |
| 3:I:93:SER:O     | 3:I:97:VAL:HG12  | 2.19                     | 0.42              |
| 3:L:96:THR:O     | 3:L:100:LEU:HG   | 2.19                     | 0.42              |
| 1:A:376:GLU:O    | 1:A:381:ARG:NH2  | 2.52                     | 0.42              |
| 3:F:115:ARG:NH2  | 3:F:151:ASP:HA   | 2.35                     | 0.42              |
| 1:J:193:ALA:HB2  | 1:J:205:ILE:HG12 | 2.01                     | 0.42              |
| 2:K:183:LEU:O    | 2:K:199:THR:N    | 2.53                     | 0.42              |
| 1:A:223:LEU:HD23 | 1:A:223:LEU:HA   | 1.83                     | 0.42              |
| 1:A:540:VAL:O    | 1:A:544:LEU:HB2  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:556:LEU:O    | 1:D:560:VAL:HG12 | 2.19                     | 0.42              |
| 3:F:88:ASP:HB2   | 3:F:118:HIS:CD2  | 2.53                     | 0.42              |
| 1:G:241:GLU:OE1  | 1:G:245:MSE:HG3  | 2.18                     | 0.42              |
| 1:G:436:VAL:O    | 1:G:439:PHE:N    | 2.53                     | 0.42              |
| 2:H:109:ASP:OD1  | 2:H:110:TRP:N    | 2.52                     | 0.42              |
| 1:J:270:LEU:O    | 1:J:274:VAL:HG23 | 2.20                     | 0.42              |
| 1:J:327:LEU:HD21 | 1:J:331:LYS:NZ   | 2.34                     | 0.42              |
| 1:J:517:THR:HA   | 1:J:521:MSE:HE2  | 2.01                     | 0.42              |
| 3:L:250:TRP:CZ2  | 3:L:286:PHE:CZ   | 3.07                     | 0.42              |
| 2:B:137:ASP:OD2  | 2:B:139:GLU:HG3  | 2.19                     | 0.42              |
| 2:E:116:TYR:CZ   | 2:E:118:GLY:HA2  | 2.54                     | 0.42              |
| 3:I:157:ALA:HB3  | 3:I:165:CYS:HB2  | 2.01                     | 0.42              |
| 3:L:5:VAL:HG12   | 3:L:6:PHE:H      | 1.84                     | 0.42              |
| 3:L:156:THR:CG2  | 3:L:166:LEU:CB   | 2.97                     | 0.42              |
| 3:L:204:ASP:OD2  | 3:L:206:ARG:HG2  | 2.19                     | 0.42              |
| 3:I:86:TYR:OH    | 3:I:114:LEU:O    | 2.33                     | 0.42              |
| 1:J:385:ILE:HD11 | 1:J:404:LEU:HD11 | 2.00                     | 0.42              |
| 2:K:30:SER:C     | 2:K:32:ASP:H     | 2.28                     | 0.42              |
| 2:K:173:ARG:HE   | 2:K:175:MET:HE3  | 1.84                     | 0.42              |
| 1:A:229:VAL:HG22 | 1:A:270:LEU:HD23 | 2.01                     | 0.42              |
| 3:C:160:ASP:CB   | 3:C:282:LEU:HD11 | 2.50                     | 0.42              |
| 1:G:552:ASP:OD2  | 1:G:554:SER:OG   | 2.38                     | 0.42              |
| 2:K:111:THR:HG22 | 2:K:187:LEU:HG   | 2.01                     | 0.42              |
| 3:L:223:ASP:OD1  | 3:L:223:ASP:N    | 2.51                     | 0.42              |
| 3:C:25:GLU:OE2   | 3:C:141:ASN:ND2  | 2.53                     | 0.42              |
| 3:F:6:PHE:CE1    | 3:F:9:GLU:HG2    | 2.52                     | 0.42              |
| 3:F:168:GLY:O    | 3:F:239:ARG:CD   | 2.61                     | 0.42              |
| 1:J:316:ASP:C    | 1:J:318:ARG:H    | 2.27                     | 0.42              |
| 1:J:384:ILE:HG23 | 1:J:385:ILE:HD12 | 2.02                     | 0.42              |
| 2:K:186:PHE:HD1  | 2:K:187:LEU:N    | 2.18                     | 0.42              |
| 3:L:45:VAL:CG1   | 3:L:156:THR:OG1  | 2.65                     | 0.42              |
| 1:D:287:PHE:CD2  | 1:D:326:ILE:HD11 | 2.54                     | 0.42              |
| 1:J:495:TYR:O    | 1:J:496:LEU:C    | 2.63                     | 0.42              |
| 2:K:207:LYS:O    | 2:K:209:TYR:N    | 2.52                     | 0.42              |
| 3:C:115:ARG:NH2  | 3:C:151:ASP:HA   | 2.35                     | 0.42              |
| 1:D:141:PHE:CE1  | 2:E:27:ILE:HD12  | 2.55                     | 0.42              |
| 2:E:183:LEU:O    | 2:E:199:THR:N    | 2.48                     | 0.42              |
| 3:F:84:GLY:O     | 3:F:116:GLY:HA3  | 2.19                     | 0.42              |
| 1:G:414:ASP:OD1  | 1:G:415:ALA:N    | 2.49                     | 0.42              |
| 3:I:61:GLN:HB3   | 3:I:64:ASP:OD2   | 2.20                     | 0.42              |
| 1:J:140:TRP:CD1  | 1:J:140:TRP:N    | 2.87                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:193:LEU:HD23 | 2:K:220:LYS:HE3  | 2.02                     | 0.42              |
| 1:A:20:LEU:HD23  | 1:A:20:LEU:HA    | 1.67                     | 0.41              |
| 1:A:32:ILE:HA    | 1:A:32:ILE:HD12  | 1.86                     | 0.41              |
| 1:A:225:VAL:HG11 | 1:A:263:VAL:HG12 | 2.02                     | 0.41              |
| 2:B:54:VAL:HG12  | 2:B:68:ASN:HB3   | 2.02                     | 0.41              |
| 2:E:175:MET:SD   | 2:E:175:MET:N    | 2.93                     | 0.41              |
| 2:H:170:VAL:HB   | 2:H:183:LEU:HD12 | 2.02                     | 0.41              |
| 2:K:203:HIS:HB2  | 2:K:210:MET:HE2  | 2.02                     | 0.41              |
| 2:B:212:ARG:NH2  | 2:B:250:GLU:OE1  | 2.45                     | 0.41              |
| 3:C:163:ILE:HG12 | 3:C:236:LEU:CD2  | 2.50                     | 0.41              |
| 1:G:537:ARG:O    | 1:G:540:VAL:HB   | 2.20                     | 0.41              |
| 1:J:6:SER:O      | 1:J:6:SER:OG     | 2.34                     | 0.41              |
| 1:J:222:LEU:HB3  | 1:J:259:VAL:HG22 | 2.01                     | 0.41              |
| 1:J:291:MSE:O    | 1:J:333:LEU:HD21 | 2.21                     | 0.41              |
| 3:C:164:PHE:HB2  | 3:C:234:LEU:HD23 | 2.02                     | 0.41              |
| 3:F:168:GLY:HA3  | 3:F:199:LEU:CA   | 2.50                     | 0.41              |
| 3:F:169:GLY:HA2  | 3:F:239:ARG:HD3  | 2.02                     | 0.41              |
| 1:G:83:PRO:HA    | 1:G:86:VAL:HG23  | 2.02                     | 0.41              |
| 2:H:193:LEU:HA   | 2:H:220:LYS:HA   | 2.02                     | 0.41              |
| 3:I:208:GLY:HA2  | 3:I:224:ILE:HD13 | 2.01                     | 0.41              |
| 1:A:370:LEU:HD23 | 1:A:370:LEU:HA   | 1.83                     | 0.41              |
| 1:D:278:ILE:O    | 1:D:282:ASP:N    | 2.38                     | 0.41              |
| 1:D:465:ASN:ND2  | 1:D:465:ASN:H    | 2.19                     | 0.41              |
| 2:E:40:LEU:O     | 2:E:41:HIS:ND1   | 2.53                     | 0.41              |
| 1:G:171:ARG:NH2  | 1:G:204:GLU:OE2  | 2.53                     | 0.41              |
| 1:G:255:LYS:HD3  | 1:G:255:LYS:HA   | 1.83                     | 0.41              |
| 1:J:76:PHE:O     | 1:J:80:VAL:HG23  | 2.21                     | 0.41              |
| 1:A:427:MSE:N    | 1:A:428:PRO:HD2  | 2.36                     | 0.41              |
| 2:B:219:SER:HB2  | 2:B:243:PRO:HD2  | 2.03                     | 0.41              |
| 3:C:54:VAL:HG13  | 3:C:276:MET:HB3  | 2.03                     | 0.41              |
| 1:D:470:VAL:O    | 1:D:474:GLY:N    | 2.40                     | 0.41              |
| 1:G:311:GLU:O    | 1:G:318:ARG:NH2  | 2.53                     | 0.41              |
| 1:G:361:THR:HG22 | 1:G:365:LEU:HD12 | 2.02                     | 0.41              |
| 1:G:406:PRO:HA   | 1:G:409:VAL:HG22 | 2.03                     | 0.41              |
| 1:J:495:TYR:O    | 1:J:499:MSE:N    | 2.35                     | 0.41              |
| 2:K:45:LEU:HB2   | 2:K:46:PRO:CD    | 2.51                     | 0.41              |
| 3:L:290:ASP:HB3  | 3:L:291:PRO:HD2  | 2.02                     | 0.41              |
| 1:A:51:LEU:O     | 1:A:55:LEU:HD12  | 2.21                     | 0.41              |
| 1:D:278:ILE:HG22 | 1:D:282:ASP:HB2  | 2.02                     | 0.41              |
| 1:D:495:TYR:HA   | 1:D:498:ARG:HB2  | 2.01                     | 0.41              |
| 2:K:46:PRO:HB3   | 2:K:158:ASP:HB2  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:53:THR:N     | 3:C:79:ASN:O     | 2.47                     | 0.41              |
| 1:G:314:SER:O    | 1:G:318:ARG:HG3  | 2.21                     | 0.41              |
| 1:G:427:MSE:HE1  | 1:G:443:LEU:HD21 | 2.02                     | 0.41              |
| 1:G:439:PHE:O    | 1:G:444:ASN:N    | 2.53                     | 0.41              |
| 1:G:440:ASP:HA   | 1:G:444:ASN:HB2  | 2.03                     | 0.41              |
| 2:H:134:ASP:OD1  | 2:H:134:ASP:N    | 2.52                     | 0.41              |
| 2:H:203:HIS:ND1  | 2:H:209:TYR:O    | 2.47                     | 0.41              |
| 3:I:22:GLN:OE1   | 3:I:136:LYS:HD2  | 2.21                     | 0.41              |
| 3:I:137:TYR:CE2  | 3:I:142:VAL:HG11 | 2.56                     | 0.41              |
| 1:J:307:LYS:HB2  | 1:J:348:VAL:HB   | 2.02                     | 0.41              |
| 1:J:456:TYR:HA   | 1:J:459:ARG:HE   | 1.86                     | 0.41              |
| 3:L:209:TRP:O    | 3:L:219:THR:HG23 | 2.21                     | 0.41              |
| 2:B:179:PHE:CE2  | 2:B:203:HIS:HB3  | 2.55                     | 0.41              |
| 3:C:157:ALA:N    | 3:C:165:CYS:O    | 2.53                     | 0.41              |
| 3:F:290:ASP:HB3  | 3:F:291:PRO:HD2  | 2.02                     | 0.41              |
| 3:I:223:ASP:N    | 3:I:223:ASP:OD1  | 2.54                     | 0.41              |
| 1:J:38:ILE:O     | 1:J:42:LEU:HD22  | 2.20                     | 0.41              |
| 1:J:561:LYS:HE2  | 1:J:583:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:438:PHE:CD1  | 1:A:438:PHE:C    | 2.99                     | 0.41              |
| 2:E:170:VAL:CG1  | 2:E:183:LEU:HD12 | 2.51                     | 0.41              |
| 1:G:205:ILE:HG13 | 1:G:208:MSE:HE2  | 2.02                     | 0.41              |
| 1:G:401:SER:OG   | 1:G:434:LEU:HD21 | 2.21                     | 0.41              |
| 3:I:52:VAL:HG22  | 3:I:79:ASN:HB3   | 2.02                     | 0.41              |
| 3:I:71:ILE:HD13  | 3:I:289:PHE:HB3  | 2.02                     | 0.41              |
| 3:I:117:ASN:OD1  | 3:I:167:HIS:NE2  | 2.54                     | 0.41              |
| 3:I:211:ILE:HD12 | 3:I:211:ILE:N    | 2.36                     | 0.41              |
| 1:J:323:MSE:HE1  | 1:J:356:LEU:HD22 | 2.02                     | 0.41              |
| 1:J:544:LEU:HG   | 1:J:564:LEU:HD21 | 2.03                     | 0.41              |
| 3:L:188:GLU:CD   | 3:L:189:VAL:H    | 2.29                     | 0.41              |
| 3:C:202:ASP:OD2  | 3:C:239:ARG:NH2  | 2.54                     | 0.41              |
| 2:E:15:PHE:HE2   | 2:E:20:LEU:HD12  | 1.85                     | 0.41              |
| 3:F:84:GLY:H     | 3:F:114:LEU:HG   | 1.86                     | 0.41              |
| 1:J:346:ALA:HB3  | 1:J:383:ASN:HB2  | 2.02                     | 0.41              |
| 3:C:205:ASP:OD1  | 3:C:205:ASP:N    | 2.49                     | 0.40              |
| 2:E:111:THR:HG22 | 2:E:189:ILE:HD11 | 2.03                     | 0.40              |
| 1:G:535:ASN:HA   | 1:G:538:PHE:CE2  | 2.56                     | 0.40              |
| 3:I:248:TYR:HA   | 3:I:258:THR:O    | 2.20                     | 0.40              |
| 2:B:158:ASP:OD1  | 2:B:160:LEU:N    | 2.54                     | 0.40              |
| 3:C:5:VAL:C      | 3:C:7:THR:N      | 2.80                     | 0.40              |
| 1:D:204:GLU:O    | 1:D:208:MSE:HE2  | 2.20                     | 0.40              |
| 1:G:176:ASP:O    | 1:G:182:ARG:NH1  | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:141:LEU:O    | 2:H:173:ARG:NH2  | 2.52                     | 0.40              |
| 2:H:179:PHE:CE2  | 2:H:203:HIS:HB3  | 2.57                     | 0.40              |
| 1:J:260:ARG:O    | 1:J:263:VAL:HG22 | 2.21                     | 0.40              |
| 1:J:318:ARG:HG3  | 1:J:319:GLU:N    | 2.36                     | 0.40              |
| 3:L:6:PHE:O      | 3:L:9:GLU:N      | 2.47                     | 0.40              |
| 1:A:86:VAL:HG11  | 1:A:119:HIS:HA   | 2.03                     | 0.40              |
| 1:A:105:ARG:HG2  | 1:A:146:SER:OG   | 2.21                     | 0.40              |
| 1:A:579:ALA:O    | 1:A:583:LEU:HD12 | 2.21                     | 0.40              |
| 3:C:158:LEU:CD1  | 3:C:161:GLY:HA2  | 2.51                     | 0.40              |
| 1:D:303:SER:HA   | 1:D:306:VAL:HG23 | 2.02                     | 0.40              |
| 1:D:409:VAL:HG12 | 1:D:446:LEU:HD21 | 2.03                     | 0.40              |
| 2:E:55:LEU:HB2   | 2:E:153:VAL:HG21 | 2.04                     | 0.40              |
| 3:F:87:VAL:HG13  | 3:F:88:ASP:H     | 1.87                     | 0.40              |
| 3:F:190:PRO:HD2  | 3:F:195:MET:HG2  | 2.03                     | 0.40              |
| 1:J:13:ILE:HD11  | 1:J:50:GLU:C     | 2.46                     | 0.40              |
| 3:L:32:CYS:O     | 3:L:36:LYS:HG3   | 2.22                     | 0.40              |
| 3:L:54:VAL:HG23  | 3:L:259:ILE:CD1  | 2.51                     | 0.40              |
| 1:D:164:ALA:HA   | 1:D:167:ARG:HE   | 1.86                     | 0.40              |
| 3:F:99:LEU:HD13  | 3:F:103:LEU:CD1  | 2.51                     | 0.40              |
| 2:K:224:LEU:O    | 2:K:227:VAL:HG22 | 2.22                     | 0.40              |
| 1:A:221:ARG:HE   | 1:A:254:ASP:CG   | 2.29                     | 0.40              |
| 1:A:278:ILE:H    | 1:A:278:ILE:HD12 | 1.85                     | 0.40              |
| 2:E:175:MET:HB3  | 2:E:176:PRO:HD2  | 2.02                     | 0.40              |
| 3:F:73:GLY:HA3   | 3:F:78:THR:OG1   | 2.22                     | 0.40              |
| 1:G:9:SER:HB3    | 1:J:59:ILE:HG13  | 2.03                     | 0.40              |
| 2:H:209:TYR:HE1  | 2:H:211:LEU:HD22 | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 580/585 (99%)   | 555 (96%)  | 25 (4%)  | 0        | 100         | 100 |
| 1   | D     | 580/585 (99%)   | 552 (95%)  | 27 (5%)  | 1 (0%)   | 43          | 73  |
| 1   | G     | 582/585 (100%)  | 554 (95%)  | 28 (5%)  | 0        | 100         | 100 |
| 1   | J     | 574/585 (98%)   | 532 (93%)  | 42 (7%)  | 0        | 100         | 100 |
| 2   | B     | 212/251 (84%)   | 198 (93%)  | 13 (6%)  | 1 (0%)   | 24          | 57  |
| 2   | E     | 211/251 (84%)   | 192 (91%)  | 17 (8%)  | 2 (1%)   | 14          | 45  |
| 2   | H     | 211/251 (84%)   | 191 (90%)  | 18 (8%)  | 2 (1%)   | 14          | 45  |
| 2   | K     | 211/251 (84%)   | 193 (92%)  | 16 (8%)  | 2 (1%)   | 14          | 45  |
| 3   | C     | 295/311 (95%)   | 269 (91%)  | 25 (8%)  | 1 (0%)   | 36          | 67  |
| 3   | F     | 292/311 (94%)   | 256 (88%)  | 30 (10%) | 6 (2%)   | 5           | 31  |
| 3   | I     | 292/311 (94%)   | 261 (89%)  | 29 (10%) | 2 (1%)   | 18          | 51  |
| 3   | L     | 292/311 (94%)   | 258 (88%)  | 32 (11%) | 2 (1%)   | 18          | 51  |
| All | All   | 4332/4588 (94%) | 4011 (93%) | 302 (7%) | 19 (0%)  | 30          | 62  |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 208 | THR  |
| 2   | E     | 208 | THR  |
| 3   | F     | 7   | THR  |
| 2   | H     | 208 | THR  |
| 3   | C     | 6   | PHE  |
| 1   | D     | 296 | ALA  |
| 3   | F     | 51  | PRO  |
| 2   | K     | 208 | THR  |
| 3   | L     | 247 | GLY  |
| 3   | I     | 291 | PRO  |
| 3   | L     | 305 | PRO  |
| 3   | F     | 263 | PRO  |
| 3   | F     | 265 | TYR  |
| 3   | I     | 13  | TRP  |
| 2   | K     | 225 | MET  |
| 3   | F     | 50  | CYS  |
| 2   | E     | 235 | PRO  |
| 2   | H     | 43  | PRO  |
| 3   | F     | 84  | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | A     | 509/497 (102%)  | 509 (100%)  | 0        | 100         | 100 |
| 1   | D     | 509/497 (102%)  | 509 (100%)  | 0        | 100         | 100 |
| 1   | G     | 511/497 (103%)  | 510 (100%)  | 1 (0%)   | 87          | 87  |
| 1   | J     | 507/497 (102%)  | 507 (100%)  | 0        | 100         | 100 |
| 2   | B     | 197/228 (86%)   | 197 (100%)  | 0        | 100         | 100 |
| 2   | E     | 196/228 (86%)   | 196 (100%)  | 0        | 100         | 100 |
| 2   | H     | 196/228 (86%)   | 196 (100%)  | 0        | 100         | 100 |
| 2   | K     | 197/228 (86%)   | 197 (100%)  | 0        | 100         | 100 |
| 3   | C     | 265/275 (96%)   | 265 (100%)  | 0        | 100         | 100 |
| 3   | F     | 261/275 (95%)   | 261 (100%)  | 0        | 100         | 100 |
| 3   | I     | 262/275 (95%)   | 261 (100%)  | 1 (0%)   | 84          | 83  |
| 3   | L     | 262/275 (95%)   | 262 (100%)  | 0        | 100         | 100 |
| All | All   | 3872/4000 (97%) | 3870 (100%) | 2 (0%)   | 88          | 89  |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 204 | GLU  |
| 3   | I     | 66  | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 312 | ASN  |
| 1   | A     | 320 | ASN  |
| 1   | A     | 360 | ASN  |
| 1   | A     | 539 | ASN  |
| 1   | A     | 553 | ASN  |
| 1   | A     | 580 | GLN  |
| 2   | B     | 203 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 240 | GLN  |
| 3   | C     | 12  | GLN  |
| 3   | C     | 139 | ASN  |
| 3   | C     | 222 | GLN  |
| 1   | D     | 30  | ASN  |
| 1   | D     | 127 | HIS  |
| 1   | D     | 237 | GLN  |
| 1   | D     | 289 | ASN  |
| 1   | D     | 364 | HIS  |
| 1   | D     | 465 | ASN  |
| 1   | D     | 520 | HIS  |
| 1   | D     | 545 | GLN  |
| 1   | D     | 557 | GLN  |
| 3   | F     | 61  | GLN  |
| 3   | F     | 222 | GLN  |
| 3   | F     | 241 | HIS  |
| 1   | G     | 233 | GLN  |
| 1   | G     | 271 | GLN  |
| 1   | G     | 289 | ASN  |
| 1   | G     | 320 | ASN  |
| 1   | G     | 360 | ASN  |
| 1   | G     | 399 | GLN  |
| 1   | G     | 433 | GLN  |
| 1   | G     | 444 | ASN  |
| 1   | G     | 535 | ASN  |
| 2   | H     | 53  | ASN  |
| 3   | I     | 44  | ASN  |
| 3   | I     | 61  | GLN  |
| 3   | I     | 139 | ASN  |
| 1   | J     | 288 | GLN  |
| 1   | J     | 304 | HIS  |
| 1   | J     | 339 | GLN  |
| 1   | J     | 433 | GLN  |
| 1   | J     | 514 | GLN  |
| 1   | J     | 539 | ASN  |
| 1   | J     | 553 | ASN  |
| 3   | L     | 44  | ASN  |
| 3   | L     | 222 | GLN  |
| 3   | L     | 249 | ASN  |
| 3   | L     | 288 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | J     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | J     | 552:ASP   | C      | 553:ASN   | N      | 5.66         |
| 1     | J     | 337:ALA   | C      | 338:ASN   | N      | 4.02         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å²)           | Q<0.9  |
|-----|-------|-----------------|--------|---------|-----|-----|--------------------|--------|
| 1   | A     | 568/585 (97%)   | -0.72  | 0       | 100 | 100 | 101, 163, 207, 237 | 0      |
| 1   | D     | 568/585 (97%)   | -0.70  | 0       | 100 | 100 | 113, 161, 197, 232 | 0      |
| 1   | G     | 570/585 (97%)   | -0.73  | 0       | 100 | 100 | 115, 179, 228, 250 | 0      |
| 1   | J     | 566/585 (96%)   | -0.64  | 0       | 100 | 100 | 104, 214, 308, 366 | 0      |
| 2   | B     | 216/251 (86%)   | -0.73  | 0       | 100 | 100 | 119, 165, 210, 228 | 0      |
| 2   | E     | 215/251 (85%)   | -0.60  | 0       | 100 | 100 | 108, 159, 224, 271 | 0      |
| 2   | H     | 215/251 (85%)   | -0.66  | 0       | 100 | 100 | 104, 148, 208, 259 | 0      |
| 2   | K     | 215/251 (85%)   | -0.63  | 0       | 100 | 100 | 108, 158, 208, 226 | 0      |
| 3   | C     | 298/311 (95%)   | -0.68  | 0       | 100 | 100 | 63, 121, 163, 232  | 1 (0%) |
| 3   | F     | 296/311 (95%)   | -0.56  | 1 (0%)  | 90  | 78  | 107, 150, 192, 236 | 0      |
| 3   | I     | 296/311 (95%)   | -0.68  | 0       | 100 | 100 | 77, 120, 165, 203  | 0      |
| 3   | L     | 296/311 (95%)   | -0.65  | 0       | 100 | 100 | 157, 203, 241, 276 | 0      |
| All | All   | 4319/4588 (94%) | -0.67  | 1 (0%)  | 100 | 100 | 63, 161, 248, 366  | 1 (0%) |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | F     | 239 | ARG  | 3.8  |

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | MN   | C     | 501 | 1/1   | 0.47 | 0.13 | 204,204,204,204            | 0     |
| 4   | MN   | L     | 501 | 1/1   | 0.64 | 0.13 | 225,225,225,225            | 0     |
| 4   | MN   | I     | 501 | 1/1   | 0.78 | 0.10 | 157,157,157,157            | 0     |
| 4   | MN   | F     | 501 | 1/1   | 0.81 | 0.10 | 181,181,181,181            | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.